http://www.cas.org/support/stngen/stndoc/properties.html

```
=> e fluoxphos/cn
E1            1     FLUOXIMESTERONE/CN
E2            1     FLUOXIN/CN
E3            0 --> FLUOXPHOS/CN
E4            1     FLUOXYDIN/CN
E5            1     FLUOXYDINE/CN
E6            1     FLUOXYMESTERONE/CN
E7            1     FLUOXYMESTERONE 3-(O-(CARBOXYMETHOXIME))/CN
E8            1     FLUOXYMESTERONE BIS(TRIMETHYLSILYL) ETHER/CN
E9            1     FLUOXYMESTERONE ENOL TRIS(TRIMETHYLSILYL) ETHER/CN
E10           1     FLUOXYPHENONIUM BROMIDE/CN
E11           1     FLUOXYPREDNISOLONE/CN
E12           1     FLUOZIM G 3KH/CN

=> e fluxphos/cn
E1            1     FLUXOMAX CRNIMO 22-1/CN
E2            1     FLUXOTAL/CN
E3            0 --> FLUXPHOS/CN
E4            1     FLUXREK 01/CN
E5            1     FLUXUM/CN
E6            1     FLUZAMIDE/CN
E7            1     FLUZINAMIDE/CN
E8            2     FLUZON/CN
E9            1     FLUZOPERINE/CN
E10           1     FLVR VAN ART 143.1/CN
E11           1     FLX 113/CN
E12           1     FLX 150/CN
http://www.cas.org/support/stngen/stndoc/properties.html

=> e "4,4,4-trifluoro-3-oxobutanoate"/cn
E1            1     4,4,4-TRIFLUORO-3-OXOBUTANAL/CN
E2            1     4,4,4-TRIFLUORO-3-OXOBUTANENITRILE/CN
E3            0 --> 4,4,4-TRIFLUORO-3-OXOBUTANOATE/CN
E4            1     4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID ETHYL ESTER/CN
E5            1     4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID N-(1-METHYL-2-PHENYL-1H-I
                    NDOL-5-YL)AMIDE/CN
E6            1     4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID N-(2-PHENYL-1H-INDOL-5-YL
                    )AMIDE/CN
E7            1     4,4,4-TRIFLUORO-3-OXOBUTYRIC ACID/CN
E8            1     4,4,4-TRIFLUORO-3-OXOBUTYRONITRILE/CN
E9            1     4,4,4-TRIFLUORO-3-PHENYL-1,2-BUTADIENE/CN
E10           1     4,4,4-TRIFLUORO-3-PHENYL-2-BUTENOIC ACID ETHYL ESTER/CN
E11           1     4,4,4-TRIFLUORO-3-TRIFLUOROMETHYLBUT-2-ENOIC ACID/CN
E12           1     4,4,4-TRIFLUORO-3-TRIFLUOROMETHYLBUTYRIC ACID/CN

=> d e4
NO L# DEFINED

=> s e4
L1            1 "4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID ETHYL ESTER"/CN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   372-31-6  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4,4-trifluoro-3-oxo-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester (6CI, 8CI)
```

```
OTHER NAMES:
CN   1-Ethoxy-4,4,4-trifluorobutane-1,3-dione
CN   4,4,4-Trifluoro-3-oxo-butyric acid ethyl ester
CN   4,4,4-Trifluoro-3-oxobutanoic acid ethyl ester
CN   4,4,4-Trifluoroacetoacetic acid ethyl ester
CN   Ethyl (trifluoroacetyl)acetate
CN   Ethyl γ,γ,γ-trifluoroacetoacetate
CN   Ethyl ω,ω,ω-trifluoroacetoacetate
CN   Ethyl 3-oxo-4,4,4-trifluorobutanoate
CN   Ethyl 4,4,4-trifluoro-3-oxobutanoate
CN   Ethyl 4,4,4-trifluoro-3-oxobutyrate
CN   Ethyl 4,4,4-trifluoroacetoacetate
CN   Ethyl 4,4,4-trifluoroacetylacetonate
CN   Ethyl trifluoroacetoacetate
CN   NSC 42739
CN   NSC 49750
MF   C6 H7 F3 O3
CI   COM
LC   STN Files:   AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CBNB,
       CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, IFICDB, IFIPAT,
       IFIUDB, PS, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, USPATOLD
         (*File contains numerically searchable property data)
     Other Sources:   EINECS**, NDSL**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)


/ Structure 1 in file .gra /


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

            783 REFERENCES IN FILE CA (1907 TO DATE)
              9 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
            785 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> e "4-chloro-3-oxobutanoate"/cn
E1          1     4-CHLORO-3-OXO-BUTYRIC ACID METHYL ESTER/CN
E2          1     4-CHLORO-3-OXOBUTANANILIDE/CN
E3          0 --> 4-CHLORO-3-OXOBUTANOATE/CN
E4          1     4-CHLORO-3-OXOBUTANOIC ACID/CN
E5          1     4-CHLORO-3-OXOBUTANOIC ACID ETHYL ESTER/CN
E6          1     4-CHLORO-3-OXOBUTANOIC ACID METHYL ESTER/CN
E7          1     4-CHLORO-3-OXOBUTANOYL CHLORIDE/CN
E8          1     4-CHLORO-3-OXOBUTYRIC ACID/CN
E9          1     4-CHLORO-3-OXOBUTYRIC ACID ETHYL ESTER/CN
E10         1     4-CHLORO-3-OXOBUTYRYL CHLORIDE/CN
E11         1     4-CHLORO-3-OXOCARDA-4,14,20(22)-TRIENOLIDE/CN
E12         1     4-CHLORO-3-PENTADECYLPHENOL/CN

=> s e5
L2          1 "4-CHLORO-3-OXOBUTANOIC ACID ETHYL ESTER"/CN

=> d l2

L2   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   638-07-3  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4-chloro-3-oxo-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Acetoacetic acid, 4-chloro-, ethyl ester (7CI, 8CI)
```

OTHER NAMES:
CN γ-Chloroacetoacetic acid ethyl ester
CN 4-Chloro acetoethylacetate
CN 4-Chloro-3-oxobutanoic acid ethyl ester
CN 4-Chloro-3-oxobutyric acid ethyl ester
CN 4-Chloroacetoacetic acid ethyl ester
CN Ethyl (chloroacetyl)acetate
CN Ethyl γ-chloroacetoacetate
CN Ethyl ω-chloroacetoacetate
CN Ethyl 3-oxo-4-chlorobutanoate
CN Ethyl 4-chloro-3-oxobutanoate
CN Ethyl 4-chloro-3-oxobutyrate
CN Etnyl 4-chloroacetoacetate
MF C6 H9 Cl O3
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, USPATOLD
      (*File contains numerically searchable property data)
    Other Sources: DSL**, EINECS**, TSCA**
      (**Enter CHEMLIST File for up-to-date regulatory information)

/ Structure 2 in file .gra /

http://www.cas.org/legal/infopolicy.html

=> s l2 near l1
MISSING OPERATOR L2 NEAR
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s l2 and l1
        1035 L2
         785 L1
L3   40 L2 AND L1

=> s l3 and hydrogenation
      183968 HYDROGENATION
        2474 HYDROGENATIONS
      184230 HYDROGENATION
                (HYDROGENATION OR HYDROGENATIONS)
L4   8 L3 AND HYDROGENATION

=> d l4 ibib abs 1-8

L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:362416 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 148:121227
TITLE: Ruthenium catalyzed asymmetric hydrogenation of α- and β-ketoesters in room temperature ionic liquids using chiral P-Phos ligand
AUTHOR(S): Xu, Lijin; Lam, Kim Hung; Ruan, Jiwu; Fan, Qinghua; Chan, Albert S. C.
CORPORATE SOURCE: Open Laboratory of Chirotechnology of the Institute of Molecular Technology for Drug Discovery and Synthesis and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong

Kong, Peop. Rep. China
SOURCE: ACS Symposium Series (2007), 950(Ionic Liquids in Organic Synthesis), 224-234
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:121227
AB Chiral dipyridyl phosphine ligand was found to be effective in the Ru-catalyzed asym. hydrogenation of α- and β-keto esters in room temperature ionic liqs. with high conversions and good to excellent enantioselectivities.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:37762 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 144:273900
TITLE: Multigram-scale asymmetric hydrogenation reactions using Ru-SYNPHOS and Ru-DIFLUORPHOS catalysts
AUTHOR(S): Jeulin, Severine; Champion, Nicolas; Dellis, Philippe; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels (UMR 7573 CNRS), Ecole Nationale Superieure de Chimie de Paris, Paris, 75231/05, Fr.
SOURCE: Synthesis (2005), (20), 3666-3671
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:273900
AB The detailed procedure for the synthesis of Ru-SYNPHOS and Ru-DIFLUORPHOS catalysts are described. These catalysts displayed high rates and are quite effective for the large-scale hydrogenation reactions of carbonyl compds., such as β-keto esters RCOCH2CO2Et (R = Me, ClCH2, F3C, Ph, PhCH2OCH2), acetylacetone and hydroxyacetone.
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1206596 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 144:107747
TITLE: Ruthenium catalyzed asymmetric hydrogenation of α- and β-keto esters in ionic liquids using chiral P-Phos ligand
AUTHOR(S): Lam, Kim Hung; Xu, Lijin; Feng, Lichun; Ruan, Jiwu; Fan, Qinghua; Chan, Albert S. C.
CORPORATE SOURCE: Open Laboratory of Chirotechnology of the Institute of Molecular Technology for Drug Discovery and Synthesis and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, Peop. Rep. China
SOURCE: Canadian Journal of Chemistry (2005), 83(6-7), 903-908
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:107747
AB Chiral dipyridylphosphine ligand was used in the Ru-catalyzed asym. hydrogenation of α- and β-keto esters in room temperature

ionic liqs. giving the corresponding α- and β-hydroxy esters with high conversions and good to excellent enantioselectivities. The catalyst was recycled by simple extraction and reused five times without loss of activity and enantioselectivity.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:626146 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 141:313992
TITLE: New developments in the synthesis of heterotopic atropisomeric diphosphines via diastereoselective aryl coupling reactions
AUTHOR(S): Madec, Jonathan; Michaud, Guillaume; Genet, Jean-Pierre; Marinetti, Angela
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, UMR 7573, ENSCP 11, Paris, 75231, Fr.
SOURCE: Tetrahedron: Asymmetry (2004), 15(14), 2253-2261 CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:313992
AB The new heterotopic atropisomeric diphosphine (R)-5,6-benzo-2,2'-bis(diphenylphosphino)-4',5',6'-trimethylbiphenyl has been prepared The key step of this synthesis is a diastereoselective, intramol. aryl-aryl coupling reaction via oxidation of a suitable, chiral diarylcuprate. The catalytic properties of the diphosphine in ruthenium promoted hydrogenations of model substrates and in rhodium promoted 1,4-addns. of boronic acids to α,β-unsatd. ketones are fully comparable to those of reference ligands such as BINAP. This seems to indicate that C2-symmetry is not a structural prerequisite for atropisomeric chiral diphosphines to obtain high enantioselectivities in 1,4-addition reactions as well as in hydrogenation reactions.
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:356392 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 141:71622
TITLE: Chiral biphenyl diphosphines for asymmetric catalysis: stereoelectronic design and industrial perspectives
AUTHOR(S): Jeulin, Severine; De Paule, Sebastien Duprat; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, Ecole Nationale Superieure de Chimie de Paris, Paris, 75231, Fr.
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(16), 5799-5804 CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:71622
GI

/ Structure 3 in file .gra /

AB Both enantiomers of the chiral diphosphines I (SYNPHOS) and II (DIFLUORPHOS) are prepared on multigram scales; the electronic and steric characteristics of I and II and of rhodium complexes derived from them are determined, compared with previous diphosphine catalysts, and correlated with their activities and enantioselectivities in the hydrogenation of ketones and olefins. I and II are prepared in five steps from 6-bromo-2,3-dihydro-1,4-benzodioxane and 5-bromo-2,2-difluorobenzodioxole, resp.; lithium-metal exchange and addition to a phosphoryl or phosphinyl chloride followed by oxidation to yield phosphine oxides, regioselective lithiation and iodination, Ullman coupling of the aryl iodides, resolution (either by acid-base resolution with di-O-benzoyl-tartaric acid or by chiral HPLC), and reduction of the phosphine oxides yields I and II in 38% and 33% overall yield, resp. The bite angles of I and II are compared to those of other common diphosphine ligands such as BINAP and MeO-BIPHEP. The structure of diastereomeric chlorohydridoruthenium complexes of (S)-II with Me acetoacetate is determined The C-O stretching frequencies of chloro(carbonyl)rhodium diphosphine complexes containing I, II, BINAP, and MeO-BIPHEP are determined as a measure of the electronic demands of the diphosphine ligands. β-Keto ester, α-keto ester, 1,3-diketone, ketone, and olefin substrates are hydrogenated in the presence of nonracemic I, II, BINAP, and MeO-BIPHEP and bis(η3-methallyl)(η4-1,5-cyclooctadienyl)ruthenium; the enantioselectivities are correlated with the steric and electronic properties of the ligands. The stereoelectronic features of the ligand and the substrate deeply influence the enantioselectivities obtained in asym. hydrogenation; whereas the steric and electronic factors for I (as in other diphosphines) correlate well, the bite angle of II does not correlate to its electronic effects in asym. hydrogenation reactions, leading to complementary hydrogenation selectivities for ligands I and II.

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:70307 CAPLUS <<LOGINID::20081224>>

DOCUMENT NUMBER: 140:253116

TITLE: Difluorphos, an electron-poor diphosphane: A good match between electronic and steric features

AUTHOR(S): Jeulin, Severine; Duprat de Paule, Sebastien; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe

CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, Ecole Nationale Superieure de Chimie de Paris, Paris, 75231, Fr.

SOURCE: Angewandte Chemie, International Edition (2004), 43(3), 320-325
CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:253116

GI

/ Structure 4 in file .gra /

AB Both enantiomers of difluorphos I were synthesized and their

stereoelectronic features were evaluated in theor. and exptl. studies. The unusual π acidity of I explains the excellent results obtained with it in ruthenium-mediated asym. hydrogenation of fluorinated β-functionalized ketones. These results are better than those obtained with other biphenyl-based diphosphines.

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:502611 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 121:102611
ORIGINAL REFERENCE NO.: 121:18339a,18342a
TITLE: purification and characterization of a novel carbonyl reductase isolated from Rhodococcus erythropolis
AUTHOR(S): Zelinski, Thomas; Peters, Joerg; Kula, Maria-Regina
CORPORATE SOURCE: Institut fuer Enzymtechnologie der Heinrich-Heine-Universitaet Duesseldorf, Forschungszentrum Juelich (KFA), Julich, 52404, Germany
SOURCE: Journal of Biotechnology (1994), 33(3), 283-92
CODEN: JBITD4; ISSN: 0168-1656
DOCUMENT TYPE: Journal
LANGUAGE: English
AB During growth on n-tetradecane a novel NADH-dependent carbonyl reductase is induced in the Gram-pos. bacterium Rhodococcus erythropolis (Peters, P., Zelinski, T. and Kula, M.R. (1992) Appl. microbiol. biotechnol. 38, 334-340). The enzyme has been purified to homogeneity using fractional pH precipitation, anion exchange chromatog. and affinity chromatog. The isoelec. point of the oxidoreductase is 4.4. The apparent mol. mass of the native enzyme is 161 kDa, that of the subunits 40 kDa as determined by SDS gel electrophoresis. A tetrameric structure of the carbonyl reductase is consistent with these results. Important biochem. data concerning the application of the reductase are: a broad pH-optimum, temperature optimum at 40° and stability at room temperature for more than 5 days. The oxidoreductase accepted as substrate aliphatic and aromatic ketones, keto esters (esters of keto carboxylic acids) and halogenated carbonyl compds. and reduced them to the corresponding hydroxyl compds. with (S)-configuration with more than 98% enantiomeric excess. The NAD+-dependent oxidation of primary alcs. was not catalyzed by the carbonyl reductase, whereas secondary alcs. and hydroxy acid esters were oxidized to the corresponding carbonyl compds. at about 10-fold slower reaction rates compared to the reduction

L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:603787 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 119:203787
ORIGINAL REFERENCE NO.: 119:36369a,36372a
TITLE: Stereodivergent synthesis of fluorinated threonine derivatives in high optical purity
AUTHOR(S): Shimizu, Makoto; Yokota, Tetsuya; Fujimori, Kouichi; Fujisawa, Tamotsu
CORPORATE SOURCE: Dep. Chem. Mater., Mie Univ., Tsu, 514, Japan
SOURCE: Tetrahedron: Asymmetry (1993), 4(5), 835-8
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:203787
AB Fluorinated 3-acetoxy-2-(methoxyimino)butyrates were resolved by lipase to give the corresponding alcs. and the acetates in high optical purity. The resolved alcs. were readily converted into mono-, di-, and

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     trifluorothreonine and allothreonine derivs. by hydrogenation of
     the methoxyimino group.
http://www.cas.org/legal/infopolicy.html

=> SAVE L4 SA577385/A
ANSWER SET L4 HAS BEEN SAVED AS 'SA577385/A'

http://www.cas.org/support/stngen/stndoc/properties.html

=> e "4,4,4-trichloro-3-hydroxybutarate"/cn
E1            1     4,4,4-TRICHLORO-2-METHYLBUTYRONITRILE/CN
E2            1     4,4,4-TRICHLORO-2-METHYLCROTONALDEHYDE/CN
E3            0 --> 4,4,4-TRICHLORO-3-HYDROXYBUTARATE/CN
E4            1     4,4,4-TRICHLORO-3-HYDROXYBUTYRIC ACID/CN
E5            1     4,4,4-TRICHLORO-3-HYDROXYBUTYRONITRILE/CN
E6            1     4,4,4-TRICHLORO-3-METHYLBUTANENITRILE/CN
E7            1     4,4,4-TRICHLORO-3-METHYLBUTYRONITRILE/CN
E8            1     4,4,4-TRICHLORO-N-(3-(3-((THIEN-2-YL)CARBONYL)PYRAZOLO(1,5-A
                    )PYRIMIDIN-7-YL)PHENYL)BUTANAMIDE/CN
E9            1     4,4,4-TRICHLOROACETOACETYL CHLORIDE/CN
E10           1     4,4,4-TRICHLOROBUTAN-1-OL/CN
E11           1     4,4,4-TRICHLOROBUTANENITRILE/CN
E12           1     4,4,4-TRICHLOROBUTYL ACETATE/CN

=> e "ethyl 4,4,4-trichloro-3-hydroxybutarate"/cn
E1            1     ETHYL 4,4,4-TRICHLORO-2-CYANOCROTONATE/CN
E2            1     ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
E3            0 --> ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTARATE/CN
E4            1     ETHYL 4,4,4-TRICHLORO-3-OXOBUTANOATE/CN
E5            1     ETHYL 4,4,4-TRICHLOROACETOACETATE/CN
E6            1     ETHYL 4,4,4-TRICHLOROBUTANOATE/CN
E7            1     ETHYL 4,4,4-TRICHLOROBUTENOATE/CN
E8            1     ETHYL 4,4,4-TRICHLOROBUTYRATE/CN
E9            1     ETHYL 4,4,4-TRIFLUORO-2-((2-HYDROXYETHYL)THIO)-3-OXOBUTANOAT
                    E/CN
E10           1     ETHYL 4,4,4-TRIFLUORO-2-BUTENOATE/CN
E11           1     ETHYL 4,4,4-TRIFLUORO-2-BUTYNECARBOXYLATE/CN
E12           1     ETHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN

=> s e2
L1            1 "ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE"/CN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   19486-93-2  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Butyric acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN   Ethyl 4,4,4-trichloro-3-hydroxybutanoate
MF   C6 H9 Cl3 O3
LC   STN Files:   BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)


/ Structure 5 in file .gra /

http://www.cas.org/legal/infopolicy.html
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```
=> s l1 and hydrogenation
            18 L1
        183968 HYDROGENATION
          2474 HYDROGENATIONS
        184230 HYDROGENATION
                 (HYDROGENATION OR HYDROGENATIONS)
L2            1 L1 AND HYDROGENATION

=> d l2

L2   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2005:393998  CAPLUS <<LOGINID::20081224>>
DN   142:429938
TI   Stereoselective catalytic hydrogenation process for the
     preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the
     corresponding 4-halo-3-oxobutyrates
PA   Lonza AG, Switz.
SO   Eur. Pat. Appl., 9 pp.
     CODEN: EPXXDW
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    --------------------   --------
PI   EP 1528053          A1     20050504    EP 2003-24865          20031031
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     AU 2004291249       A1     20050602    AU 2004-291249         20041022
     CA 2541716          A1     20050602    CA 2004-2541716        20041022
     WO 2005049545       A1     20050602    WO 2004-EP11971        20041022
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     EP 1682481          A1     20060726    EP 2004-790763         20041022
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     CN 1874989          A      20061206    CN 2004-80032075       20041022
     BR 2004016133       A      20070102    BR 2004-16133          20041022
     JP 2007509874       T      20070419    JP 2006-537143         20041022
     KR 2006095769       A      20060901    KR 2006-708041         20060426
     NO 2006002131       A      20060530    NO 2006-2131           20060512
     IN 2006DN03081      A      20070810    IN 2006-DN3081         20060529
     US 20070078279      A1     20070405    US 2006-577385         20060703
PRAI EP 2003-24865       A      20031031
     WO 2004-EP11971     W      20041022
OS   CASREACT 142:429938; MARPAT 142:429938
RE.CNT  5     THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
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YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y
L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   19486-93-2  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Butyric acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN   Ethyl 4,4,4-trichloro-3-hydroxybutanoate
MF   C6 H9 Cl3 O3
LC   STN Files:   BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)
DT.CA  CAplus document type:  Journal; Patent
RL.P   Roles from patents:  PREP (Preparation); USES (Uses)
RL.NP  Roles from non-patents:  PREP (Preparation); PRP (Properties); RACT
       (Reactant or reagent); NORL (No role in record)


/ Structure 6 in file .gra /
REFERENCE  1

AN   142:429938  CA <<LOGINID::20081224>>
TI   Stereoselective catalytic hydrogenation process for the preparation of
     (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding
     4-halo-3-oxobutyrates
PA   Lonza AG, Switz.
SO   Eur. Pat. Appl., 9 pp.
     CODEN: EPXXDW
DT   Patent
LA   English
IC   ICM  C07C067-31
     ICS  C07C069-675
CC   23-17 (Aliphatic Compounds)
     Section cross-reference(s): 67
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
PI   EP 1528053         A1   20050504       EP 2003-24865    20031031
        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     AU 2004291249      A1   20050602       AU 2004-291249   20041022
     CA 2541716         A1   20050602       CA 2004-2541716  20041022
     WO 2005049545      A1   20050602       WO 2004-EP11971  20041022
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
            SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
            SN, TD, TG
     EP 1682481         A1   20060726       EP 2004-790763   20041022
        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     CN 1874989         A    20061206       CN 2004-80032075 20041022
     BR 2004016133      A    20070102       BR 2004-16133    20041022
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	JP	2007509874	T	20070419	JP 2006-537143	20041022
	KR	2006095769	A	20060901	KR 2006-708041	20060426
	NO	2006002131	A	20060530	NO 2006-2131	20060512
	IN	2006DN03081	A	20070810	IN 2006-DN3081	20060529
	US	20070078279	A1	20070405	US 2006-577385	20060703
PRAI	EP	2003-24865	20031031			
	WO	2004-EP11971	20041022			

GI

/ Structure 7 in file .gra /

AB Enantiomerically pure (S)- or (R)-4-halo-3-hydroxybutyrates [I; II; R1 = CH2X, CHX2, CX3; X = Cl and/or Br; R2 = C1-6 alkyl, C3-8 cycloalkyl, (un)substituted aryl, (un)substituted aralkyl; e.g., Et (3S)-4-chloro-3-hydroxybutyrate] are prepared in high yield and selectivity by the asym. hydrogenation of 4-halo-3-oxobutyrate esters R1C(:O)CH2CO2R2 (e.g., Et 4-chloro-3-oxobutyrate) in the presence of a catalyst of a ruthenium complex comprising a chiral diphosphine ligand (III).

ST chiral halohydroxybutyrate ester prepn stereoselective catalytic hydrogenation halooxobutyrate; asym ethyl chlorohydroxybutyrate prepn stereoselective catalytic hydrogenation chlorooxobutyrate

IT Alcohols, uses
RL: NUU (Other use, unclassified); USES (Uses)
(C1-4, solvents; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates using)

IT Carboxylic acids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(esters, chiral 4-halo-3-hydroxybutyrates; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT Stereochemistry
(stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT Hydrogenation catalysts
(stereoselective, ruthenium complex comprising a chiral diphosphine ligand; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT Hydrogenation
(stereoselective; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT 10049-08-8, Ruthenium trichloride 52462-29-0 503538-69-0 503538-70-3
RL: CAT (Catalyst use); USES (Uses)
(in a stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT 1333-74-0, Hydrogen, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(in a stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT 67-68-5, Dmso, uses 68-12-2, Dmf, uses 75-05-8, Acetonitrile, uses
RL: NUU (Other use, unclassified); USES (Uses)

(solvent; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates using)

IT 638-07-3, Ethyl 4-chloro-3-oxobutyrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT 19486-93-2P 86728-85-0P 90866-33-4P 125537-59-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates)

IT 3702-98-5 74530-56-6, tert-Butyl 4-chloro-3-oxobutyrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates using)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

(1) Duprat de Paule Sebastien; WO 03029259 A 2003
(2) Pai, C; TETRAHEDRON LETTERS 2002, V43(15), P2789 CAPLUS
(3) Takasago Perfumery Co Ltd; EP 0295109 A 1988 CAPLUS
(4) Takasago Perfumery Co Ltd; EP 0339764 A 1989 CAPLUS
(5) Takasago Perfumery Co Ltd; EP 1176135 A 2002 CAPLUS

REFERENCE 2

AN 137:369737 CA <<LOGINID::20081224>>

TI Stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors

IN Tada, Kenichi; Miura, Takashi
PA Takasago International Corporation, Japan

SO Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C07C067-317
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 67

FAN.CNT 13

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1258470	A2	20021120	EP 2002-291172	20020510
	EP 1258470	A3	20030813		
	EP 1258470	B1	20050817		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003034665	A	20030207	JP 2002-82865	20020325
	JP 4015450	B2	20071128		
	ES 2247280	T3	20060301	ES 2002-291172	20020510
	US 20030004362	A1	20030102	US 2002-142983	20020513
	US 6723871	B2	20040420		
PRAI	JP 2001-150012	20010518			
	JP 2002-82865	20020325			

GI

/ Structure 8 in file .gra /

AB Optically active β-hydroxycarboxylate esters R1CH(OH)CH2CO2R2 [R1 =

C1-10 (un)branched perfluoroalkyl or perchloroalkyl; R2 = C1-8 lower alkyl, (un)substituted benzyl; e.g., optically active Et 4,4,4-trifluoro-3-hydroxybutanoate] are prepared in high yield and selectivity by stereoselective hydrogen transfer to the corresponding β-ketocarboxylate esters R1COCH2CO2R2 (e.g., Et 4,4,4-trifluoro-3-oxobutanoate) in the presence of hydrogen donors (e.g., formic acid-triethylamine mixts.) and a chiral ruthenium-diamine complex catalyst [I; * = asym. carbon atom; R3, R4 = alkyl, Ph, (un)substituted cycloalkyl; R5 = methanesulfonyl, trifluoromethanesulfonyl, benzenesulfonyl, (un)substituted naphthyl, camphorsulfonyl, alkoxycarbonyl, (un)substituted benzoyl; R6 = H, alkyl; A = (un)substituted aromatic compound; X = halogen; e.g., RuCl[(1R,2R)-p-TsNHCH(C6H5)CH(C6H5)NH2] (p-cymene)].

ST stereoselective hydrogen transfer optically active hydroxycarboxylate ester prepn; chiral ruthenium diamine complex catalyst stereoselective hydrogen transfer; optically active ethyl trifluorohydroxybutanoate prepn stereoselective hydrogen transfer

IT Esters, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydroxy, chiral β-hydroxycarboxylate esters; stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT Esters, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(keto, β-ketocarboxylate esters; stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT Stereochemistry
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT Hydrogen transfer catalysts
(stereoselective, chiral ruthenium-diamine complex; chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT Hydrogen transfer
(stereoselective; stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT 192139-92-7
RL: CAT (Catalyst use); USES (Uses)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT 372-31-6, Ethyl 4,4,4-trifluoro-3-oxobutanoate 3702-98-5, Ethyl 4,4,4-trichloro-3-oxobutanoate 83643-84-9, Methyl 4,4,4-trifluoro-3-oxobutanoate 175230-50-9, Isopropyl 4,4,4-trifluoro-3-oxobutanoate 475467-54-0, Methyl 3-oxo-4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-pentadecafluorodecanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT 64-18-6, Formic acid, reactions 75-50-3, Trimethylamine, reactions

RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

IT 372-30-5P, Ethyl 4,4,4-trifluoro-3-hydroxybutanoate 19486-93-2P, Ethyl 4,4,4-trichloro-3-hydroxybutanoate 305322-80-9P, Isopropyl 4,4,4-trifluoro-3-hydroxybutanoate 475467-53-9P, Methyl 4,4,4-trifluoro-3-hydroxybutanoate 475467-55-1P, Methyl 3-hydroxy-4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-pentadecafluorodecanoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

REFERENCE 3

AN 100:22738 CA <<LOGINID::20081224>>
TI Heterosubstituted (silicon, germanium) 2-oxetanones. Reaction of silyl- and germylketenes with polyfluorinated ketones and properties of 3-silyl(germyl)-2-oxetanones
AU Zaitseva, G. S.; Livantsova, L. I.; Bekker, R. A.; Baukov, Yu. I.; Lutsenko, I. F.
CS Mosk. Gos. Univ., Moscow, USSR
SO Zhurnal Obshchei Khimii (1983), 53(9), 2068-77
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Russian
CC 29-8 (Organometallic and Organometalloidal Compounds)
GI

/ Structure 9 in file .gra /

AB Reaction of silyl- and germylketenes (e.g., Me3SiCH:CO) with polyfluorinated ketones [e.g., (CF3)3CO] gave a mixture of 1:1 cycloadducts (2-oxetanones, e.g., I) and 2:1 cyclodimers, e.g., II. Some reactions of the oxetanones were studied.
ST ketone polyfluoro cycloaddn ketene; silylketene cycloaddn polyfluoro ketone; germylketene cycloaddn polyfluoro ketone; oxetanone silyl germyl
IT Cycloaddition reaction
(of silyl- and germylketenes with polyfluorinated ketones)
IT 79305-64-9P 83740-52-7P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and reaction of, with (trimethylsilyl)ketene)
IT 67354-06-7P 67354-19-2P 67354-21-6P 67354-23-8P 67354-24-9P 67354-25-0P 67354-26-1P 88237-28-9P 88237-29-0P 88237-30-3P 88237-31-4P 88237-32-5P 88237-33-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)
IT 4964-02-7P 4964-03-8P 4964-04-9P 4964-05-0P 13159-46-1P 19486-93-2P 24099-72-7P 56183-55-2P 56183-56-3P 62019-87-8P 67354-12-5P 67354-13-6P 67354-15-8P 67354-16-9P 67354-17-0P 67354-18-1P 75668-12-1P 80673-03-6P 88237-34-7P 88237-35-8P 88237-36-9P 88237-37-0P 88237-38-1P 88237-39-2P 88237-40-5P 88237-41-6P 88237-42-7P 88237-43-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 127-21-9 421-50-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ketenes)
IT 64-17-5, reactions 109-89-7, reactions 121-44-8, reactions 124-40-3, reactions 2083-91-2 7727-15-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with oxetanones)
IT 4071-85-6 32278-84-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with polyfluorinated ketones)

REFERENCE 4

AN 96:68256 CA <<LOGINID::20081224>>
TI New syntheses of trichloromethyl functional alcohols. Studies of their tranquilizing properties
AU Deleris, Gerard; Dunogues, Jacques; Babin, Pierre; Calas, Raymond; Bardone, Marie Claude; Guyonnet, Jean Claude
CS Lab. Chim. Org. Composes Org. Silicium Etain, CNRS, Talence, 33405, Fr.
SO European Journal of Medicinal Chemistry (1981), 16(6), 533-7
CODEN: EJMCA5; ISSN: 0009-4374
DT Journal
LA French
CC 23-7 (Aliphatic Compounds)
Section cross-reference(s): 1
AB CCl3CHROH (I, R = BuC.tplbond.C, Me3SiC.tplbond.C, Me3SiCH2C.tplbond.C, PhC.tplbond.C, 3-pyridylethynyl, EtO2CCH2, Et2NCOCH2, 2-pyridyl) were prepared by treating RSiMe3 with chloral, and methanolysis of Cl3CCHROSiMe3. I(R = Et2NCOCH2, 2-pyridyl) had tranquilizing activity comparable to that of meprobamate, the pyridine derivative being free of convulsant side-effects.
ST trichlorobutynol prepn tranquilizer
IT Tranquilizers and Neuroleptics
(trichlorobutynols)
IT 57212-16-5P 57212-18-7P 57212-20-1P 80673-03-6P 80673-04-7P 80673-05-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of)
IT 25290-15-7P 57212-17-6P 57212-19-8P 57212-21-2P 80673-02-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and pharmacol. activity of)
IT 2170-06-1P 3844-94-8P 4071-88-9P 13737-04-7P 14630-40-1P 21752-80-7P 23138-65-0P 80673-00-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with chloral)
IT 6181-26-6P 19486-93-2P 80673-01-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 75-87-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with trimethylsilylalkynes)
IT 105-39-5 109-04-6 127-18-4, reactions 536-74-3 627-41-8 693-02-7 1121-55-7 2315-36-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation of)

REFERENCE 5

AN 95:2477 CA <<LOGINID::20081224>>
TI Latent inhibitors. Part 2. Allylic inhibitors of alcohol dehydrogenase
AU MacInnes, Iain; Schorstein, David E.; Suckling, Colin J.; Wrigglesworth, Roger
CS Dep. Pure Appl. Chem., Univ. Strathclyde, Glasgow, G1 1XL, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1981), (4), 1103-8
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
CC 7-3 (Enzymes)
AB Of a number of 3-substituted prop-2-en-1-ols and -1-als tested for latent inhibition of horse liver alc. dehydrogenase (EC 1.1.1.1), only 3-ethylthioprop-2-en-1-ol was active, via oxidation to the corresponding aldehyde catalyzed by the enzyme. Product studies and kinetic detns. indicated that the persistence of inhibition was due to EtSH, formed by an enzyme-catalyzed hydrolysis of the aldehyde. The preparation of the inhibitors is described.
ST liver alc dehydrogenase propenol propenal
IT Liver, composition
(alc. dehydrogenase of, propenols and propenals latent inhibition of)
IT 107-18-6, biological studies 107-19-7 16263-71-1 37675-33-5 56772-86-2 67935-24-4 77889-97-5 77889-98-6 77889-99-7 77890-00-7 77890-97-2 77890-98-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(alc. dehydrogenase of liver response to)
IT 623-47-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)
IT 9031-72-5
RL: PROC (Process)
(of liver, propenols and propenals latent inhibition of)
IT 77890-03-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidative deethylation of)
IT 2579-22-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(phenoxylation of)
IT 19486-93-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
IT 13001-71-3P 42844-38-2P 77890-01-8P 77890-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 75-87-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et bromoacetate)
IT 75-08-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et propiolate)
IT 105-36-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloral)
IT 624-67-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethanethiol)
IT 75-89-8 100-02-7, reactions 108-95-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with phenylpropynal)
IT 504-17-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tetraethoxypropane)
IT 122-31-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thiobarbituric acid)
IT 2579-22-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with trifluoroethanol)

REFERENCE 6

AN 94:22995 CA <<LOGINID::20081224>>
TI Pressure- or heat-sensitive recording material
IN Petitpierre, Jean Claude
PA Ciba-Geigy A.-G., Switz.
SO Ger. Offen., 30 pp.
CODEN: GWXXBX
DT Patent
LA German
IC B41M005-12; B41M005-18
CC 74-8 (Radiation Chemistry, Photochemistry, and Photographic Processes)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2946830	A1	19800529	DE 1979-2946830	19791120
	DE 2946830	C2	19811029		
	US 4291901	A	19810929	US 1979-95119	19791116
	EP 12112	A1	19800611	EP 1979-810160	19791119
	EP 12112	B1	19831005		
	R: AT, BE, CH, DE, FR, GB, IT				
	FI 7903646	A	19800524	FI 1979-3646	19791121
	CA 1139559	A1	19830118	CA 1979-340288	19791121
	JP 55073586	A	19800603	JP 1979-152367	19791122
	JP 63043236	B	19880829		
	FR 2442139	A1	19800620	FR 1979-28857	19791122
	FR 2442139	B1	19810227		
	BR 7907589	A	19800805	BR 1979-7589	19791122
	GB 2047417	A	19801126	GB 1979-40479	19791122
	GB 2047417	B	19830420		
PRAI	CH 1978-12026		19781123		
	CH 1979-9628		19791026		

AB Pressure- or heat-sensitive recording materials using a system composed of a reactive combination of a color developer and a color former contain a compound of the general formula RCHOHZR1m (R = a reactive organic methylene or Me compound, R2R3N, R1mZ1CHOHNR4NZ2NR2, or R5S where R2, R3, R4 = H, substituted or unsubstituted alkyl, aralkyl, alkanoyl, alkylsulfonyl, aroyl, arylsulfonyl, cyanoamidino, substituted carbamoyl, or substituted sulfamoyl; Z1 = alkylene, arylene, or aralkylene; Z2 = CO, SO2 COCO, substituted carbonylmethylenecarbonyl, alkylene, or phenylene; R5 = substituted or unsubstituted alkyl, aralkyl, aryl, or a 5-membered heterocycle; R1 = halogen, CN, or NO2; Z = same as Z1; m = 1-6) as the color developer. Thus, a mixture containing PhNHCONHCHOHCC13 32, the distearylamide of ethylenediamine 3.8, kaolin 39, poly(vinyl alc) (88% hydrolyzed) 20 g, and water 500 mL was ball-milled to a particle size of 5 μ. In a 2nd ball mill was milled a mixture of 2-phenylamino-3-methyl-6-diethylaminofluoran 6, poly(vinyl alc.) (88% hydrolyzed) 3, and water 60 mL to give a particle size of .apprx.3 μ. Both dispersion were then combined and cooled at 5.5 g/m2 on a paper support. Application of a heated ball-point pen to the paper gave an

intense black color that had excellent lightfastness.
ST color developer pressure thermal recording; thermal recording color developer; copying pressure sensitive color developer; urea deriv color developer copying
IT Thermography
(heat-sensitive compns. for, containing urea derivs. as color developers)
IT Copying paper
(pressure-sensitive, color developers for, urea derivs. as)
IT 57-13-6D, derivs. 116-52-9 760-40-7 1552-33-6 5445-85-2
6316-07-0 13505-41-4 15446-11-4 19177-72-1 19486-93-2 31339-87-4
33243-78-6 42840-67-5 53376-31-1 54888-09-4 69796-31-2
75456-90-5 75456-91-6 75456-92-7 75456-93-8 75456-94-9
75456-95-0 75456-96-1 75456-97-2 75456-98-3 75456-99-4
75457-00-0 75457-01-1 75457-02-2 75457-03-3 75457-04-4
75457-05-5 75457-06-6 75457-07-7 75457-08-8
RL: USES (Uses)
(color developer, for pressure- or heat-sensitive recording materials)
IT 110-30-5 1552-42-7 29512-49-0
RL: USES (Uses)
(pressure-sensitive copying materials containing urea derivative color developer and)

REFERENCE 7

AN 87:52713 CA <<LOGINID::20081224>>
TI Reaction of chloral with ortho esters and acetaldehyde acetal
AU Petrov, K. A.; Tikhonova, N. A.; Shchekotikhina, N. A.
CS USSR
SO Zhurnal Organicheskoi Khimii (1977), 13(5), 939-43
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
CC 23-17 (Aliphatic Compounds)
AB Cl3CHO (I) reacted with HC(OEt)3 containing H2SO4, dry HCl or ZnCl2 to give Cl3CCH(OH)OEt (II) and Cl3CCH(OEt)2. Treating II with MeC(OEt)3 in C6H6 containing ZnCl2 at 120° yielded 12.5% Cl3CCH(OH)CH2CO2Et and 56.5% Cl3CCH:CHCO2Et. I reacted with RC(OR1)3 (R = H, R1 = Me, Et; R = EtO, R1 = Et) containing NaOAc to give 50-70% Cl3CCH(OR1)OCR(OR1)2 (III). Alcoholysis of III (R = H, R1 = Me, Et) gave up to quant. yields of Cl3CCH(OH)OR1 and HC(OR1)3. Reacting I with MeCH(OEt)2 gave 25% Cl3CCH(OEt)OCHMeOEt in the absence of catalyst and CH2:CHOEt and II in quant. yield in the presence of anhydrous NaOAc.
ST chloral reaction ortho ester acetal
IT 63504-87-0P 63504-89-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alcoholysis of)
IT 515-83-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ethyl orthoformate)
IT 109-92-2P 599-97-3P 2791-89-1P 13001-71-3P 19486-93-2P
63504-88-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 105-57-7 122-51-0 149-73-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloral)
IT 78-39-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloral hydrate)
IT 302-17-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl orthoacetate)
IT 75-87-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ortho esters and with acetaldehyde diethyl acetal)

REFERENCE 8

AN 75:42672 CA <<LOGINID::20081224>>
TI Spectroscopic study of an intramolecular hydrogen bond in hydroxycarboxylic acids and their esters
AU Abramovich, M. A.; Ginzburg, I. M.; Ioffe, D. V.
CS Leningr. Khim.-Farm. Inst., Leningrad, USSR
SO Teoreticheskaya i Eksperimental'naya Khimiya (1971), 7(2), 225-31
CODEN: TEKHA4; ISSN: 0497-2627
DT Journal
LA Russian
CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
AB Frequencies of stretching vibrations (ν) of OH and CO groups of 10 hydroxycarboxylic acids and their esters (CCl4 solns.) were studied with respect to the formation of intramol. H bonds. Effect of substituents on the strength of the H bonds and, therefore, on ν is discussed.
ST hydroxy carboxylic acid hydrogen bond; IR hydroxy carboylic acid
IT Hydrogen bonds
(in hydroxycarboxylic acids, ir spectra in relation to)
IT Spectra, infrared
REFERENCE 9

AN 74:76484 CA <<LOGINID::20081224>>
TI Organotin compounds. XXIII. Reformatsky-type reactions with α-functionally substituted organotin compounds
AU Noltes, Jan G.; Verbeek, F.; Creemers, Henricus M. J. C.
CS Inst. Org. Chem., TNO, Utrecht, Neth.
SO Organometallics in Chemical Synthesis (1970), Volume Date 1970-1971, 1, 57-68
CODEN: OMCSAW; ISSN: 0030-5162
DT Journal
LA English
CC 29 (Organometallic and Organometalloidal Compounds)
AB α-Functionally substituted organotin compds. R3SnCH2X add across the carbonyl group of aldehydes and ketones R1R2C:O to give the corresponding β-triorganostannoxy-substituted-carbon-functional compds. R3SnOCR1R2CH2X. Based on the observed substituent effects and on kinetic measurements these reactions proceed by an ionic mechanism involving nucleophilic attack on the carbonyl C atom as the rate-determining step. In view of the ease of fission of the Sn-O bond of the stannoxy adducts by mineral or organic acids (cleavage by malonic or oxalic acid is the preferred method) this reaction offers an attractive route to β-hydroxysubstituted-carbon-functional compds. of the type HOCR1R2CH2X (R1 = organic group or H). Starting from the appropriate organotin nitriles (X = CN), esters (X = CO2Et), ketones (X = Ac) and amides (X = CONEt2) a variety of β-hydroxynitriles, -esters, -ketones and -amides were prepared NMR spectroscopy offers a useful tool to follow the progress of the addition reactions. Representative NMR data for some organotin adducts and for the corresponding β-hydroxy-substituted-carbon-functional compounds are given. The synthesis of 18 new β-hydroxy compds. of the type HOCR1R2CH2X is presented as an example to illustrate the synthetic utility of this reaction sequence.
ST tin org compd; Reformatskii reaction organotin

IT Aldehydes, reactions
Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with trialkylstannane derivs.)
IT Kinetics of addition reactions
(of carbonyl compds. with trialkylstannane derivs.)
IT Addition reactions
(of carbonyl compds. with trialkylstannane derivs., mechanism of)
IT 997-50-2D, Stannane, triethyl-, derivs. 14230-31-0 14230-36-5
17729-59-8 31602-69-4 31775-87-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with carbonyl compds.)
IT 1029-92-1 5381-93-1 17226-70-9 17981-09-8 17981-12-3 17981-13-4
17981-16-7 17981-17-8 17981-18-9 17981-25-8 19486-93-2
30543-30-7, 5-Hexen-2-one, 4-[(triethylstannyl)oxy]-
RL: PRP (Properties)
(nuclear magnetic resonance of)
IT 6050-51-7P 7466-48-0P 7497-61-2P 17981-24-7P 19487-29-7P
25290-13-5P 25290-14-6P, 2-Heptanone, 4-hydroxy- 25290-15-7P
25290-16-8P 25290-18-0P 25290-19-1P 25290-20-4P 25290-21-5P,
2-Furanhydracrylic acid, methyl ester 30543-15-8P, 2-Butanone,
4-(o-chlorophenyl)-4-hydroxy- 30543-21-6P, 2-Propanone,
1-(1-hydroxy-1-indanyl)- 30543-32-9P, Hydrocinnamic acid,
β,β'-[(diethylstannylene)dioxy]bis-, dimethyl ester
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

REFERENCE 10

AN 71:101296 CA <<LOGINID::20081224>>
TI Alcohols
IN Cremers, Henricus M. J. C.; Noltes, Jan G.
PA Nederlandse Centrale Organisatie voor Toegepast-Natuurwetenschappelijk Onderzoek
SO Ger. Offen., 22 pp.
CODEN: GWXXBX
DT Patent
LA German
IC C07BCD
CC 23 (Aliphatic Compounds)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 1816282		19690717	DE 1968-1816282	19681221
NL 6800090			NL	
NL 6816868			NL	
PRAI NL	19680103			
NL	19681126			

AB The title compds. were prepared by reacting an organotin compound with a ketone or thioketone followed by mild hydrolysis. Thus, 1.5 g. pentafluorobenzaldehyde was treated with Bu3SnCH2CN at room temperature 16 hrs. followed by addition of 2 ml. absolute Et2O and 161 mg. HCl dissolved in absolute
Et2O to give 63% C6F5CH(OH)CH2CN, m. 88-9°. The following compds. were similarly prepared (comp. and properties given): Cl3CCH(OH)CH2CO2Et, m. 54.5-5.5°; PrCH(OH)CH2COMe, b0·04 40°, n20D 1.4343; PhCH(OH)CH2C(OH)Me, b0·09 90-2°, n20D 1.5264; p-O2NC6H4CH(OH)CH2C(O)Me, -; RCH(OH)CH2COMe (R = 2-furyl), b0·07 76-8°; n20D 1.4923; (ClCH2)2C(OH)CH2COMe, 61-2°, n20D 1.4829; 1-acetylmethylcyclopentanol, b0·03-0·05 48-b0·05 50°; 1-acetylmethylcyclohexanol, n20D 1.4701;

C13CCH(OH)CH2CONEt2, m. 63-5°; C6F5CH(OH)CH2C(O)NEt2, m. 66-7.5°; RCH(OH)CH2CO NEt2 (R = 2-furyl), b0·2 128-32°, n20D 1.5302; PhCMe(OH)C H2COMe, b0·07 68-78° n20D 1.5530; PhCH(OH)CH2CONEt2, n20D 1.5265; N,N-diethyl-(1-hydroxycyclopentyl)acetamide, -; PhCH(OH)CH2CN, -; RCH(OH)CH2CN (R = 2-furyl), -; RCH(OH)CH2CO2Et (R = 2-furyl), -; p-O2N C6H4CH(OH)CH2CO2Et, -.

ST hydroxy ketone; ketone hydroxy; amides hydroxy; ester hydroxy; nitriles hydroxy; organo tins ketone; tins organo ketone

IT Alcohols, preparation
RL: PREP (Preparation)
(from carbonyl compds. by reaction with organic tin compds.)

IT Carbonyl compounds, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with organic tin compds., alcs. by)

IT 38134-31-5P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Alcohols)

IT 5381-93-1P 6050-51-7P 7497-61-2P 15121-66-1P 17981-09-8P
17981-10-1P 17981-11-2P 17981-12-3P 17981-13-4P 17981-24-7P
19486-93-2P 19487-29-7P 25290-13-5P 25290-14-6P 25290-15-7P
25290-16-8P 25290-17-9P 25290-18-0P 25290-19-1P 25290-20-4P
25290-21-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 7440-31-5, Tin
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of organic, with carbonyl compds.)

ACCESSION NUMBER: 142:429938 CA <<LOGINID::20081224>>
TITLE: Stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrates
PATENT ASSIGNEE(S): Lonza AG, Switz.
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1528053	A1	20050504	EP 2003-24865	20031031
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004291249	A1	20050602	AU 2004-291249	20041022
CA 2541716	A1	20050602	CA 2004-2541716	20041022
WO 2005049545	A1	20050602	WO 2004-EP11971	20041022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1682481	A1	20060726	EP 2004-790763	20041022

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        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     CN 1874989        A    20061206       CN 2004-80032075 20041022
     BR 2004016133     A    20070102       BR 2004-16133    20041022
     JP 2007509874     T    20070419       JP 2006-537143   20041022
     KR 2006095769     A    20060901       KR 2006-708041   20060426
     NO 2006002131     A    20060530       NO 2006-2131     20060512
     IN 2006DN03081    A    20070810       IN 2006-DN3081   20060529
     US 20070078279    A1   20070405       US 2006-577385   20060703
PRIORITY APPLN. INFO.:                     EP 2003-24865    20031031
                                           WO 2004-EP11971  20041022
GI


/ Structure 10 in file .gra /


AB   Optically active β-hydroxycarboxylate esters R1CH(OH)CH2CO2R2 [R1 =
     C1-10 (un)branched perfluoroalkyl or perchloroalkyl; R2 = C1-8 lower
     alkyl, (un)substituted benzyl; e.g., optically active Et
     4,4,4-trifluoro-3-hydroxybutanoate] are prepared in high yield and
     selectivity by stereoselective hydrogen transfer to the corresponding
     β-ketocarboxylate esters R1COCH2CO2R2 (e.g., Et
     4,4,4-trifluoro-3-oxobutanoate) in the presence of hydrogen donors (e.g.,
     formic acid-triethylamine mixts.) and a chiral ruthenium-diamine complex
     catalyst [I; * = asym. carbon atom; R3, R4 = alkyl, Ph, (un)substituted
     cycloalkyl; R5 = methanesulfonyl, trifluoromethanesulfonyl,
     benzenesulfonyl, (un)substituted naphthyl, camphorsulfonyl,
     alkoxycarbonyl, (un)substituted benzoyl; R6 = H, alkyl; A =
     (un)substituted aromatic compound; X = halogen; e.g.,
     RuCl[(1R,2R)-p-TsNHCH(C6H5)CH(C6H5)NH2] (p-cymene)].
http://www.cas.org/legal/infopolicy.html

=> activate SA2577385/A
L1  (         1)SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  "ETHYL 4,4,4-TRICHLOR
L2            1 SEA FILE=CAPLUS SPE=ON  ABB=ON  PLU=ON  L1 AND HYDROGENATION

=> d ibib abs l2

L2   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2005:393998  CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER:          142:429938
TITLE:                    Stereoselective catalytic hydrogenation
                          process for the preparation of (S)- or
                          (R)-4-halo-3-hydroxybutyrate esters from the
                          corresponding 4-halo-3-oxobutyrates
PATENT ASSIGNEE(S):       Lonza AG, Switz.
SOURCE:                   Eur. Pat. Appl., 9 pp.
                          CODEN: EPXXDW
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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     EP 1528053           A1    20050504    EP 2003-24865          20031031
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     AU 2004291249        A1    20050602    AU 2004-291249         20041022
     CA 2541716           A1    20050602    CA 2004-2541716        20041022
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     WO 2005049545        A1    20050602    WO 2004-EP11971        20041022
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              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
              SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
     EP 1682481           A1    20060726    EP 2004-790763         20041022
          R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     CN 1874989           A     20061206    CN 2004-80032075       20041022
     BR 2004016133        A     20070102    BR 2004-16133          20041022
     JP 2007509874        T     20070419    JP 2006-537143         20041022
     KR 2006095769        A     20060901    KR 2006-708041         20060426
     NO 2006002131        A     20060530    NO 2006-2131           20060512
     IN 2006DN03081       A     20070810    IN 2006-DN3081         20060529
     US 20070078279       A1    20070405    US 2006-577385         20060703
PRIORITY APPLN. INFO.:                      EP 2003-24865       A  20031031
                                            WO 2004-EP11971     W  20041022
OTHER SOURCE(S):          CASREACT 142:429938; MARPAT 142:429938
GI
/ Structure 11 in file .gra /


AB   Enantiomerically pure (S)- or (R)-4-halo-3-hydroxybutyrates [I; II; R1 =
     CH2X, CHX2, CX3; X = Cl and/or Br; R2 = C1-6 alkyl, C3-8 cycloalkyl,
     (un)substituted aryl, (un)substituted aralkyl; e.g., Et
     (3S)-4-chloro-3-hydroxybutyrate] are prepared in high yield and selectivity
     by the asym. hydrogenation of 4-halo-3-oxobutyrate esters
     R1C(:O)CH2CO2R2 (e.g., Et 4-chloro-3-oxobutyrate) in the presence of a
     catalyst of a ruthenium complex comprising a chiral diphosphine ligand
     (III).
REFERENCE COUNT:          5     THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> activate SA577385/A
L3  (         1)SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  "4,4,4-TRIFLUORO-3-OX
L4  (         1)SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  "4-CHLORO-3-OXOBUTANO
L5  (        40)SEA FILE=CAPLUS SPE=ON  ABB=ON  PLU=ON  L4 AND L3
L6             8 SEA FILE=CAPLUS SPE=ON  ABB=ON  PLU=ON  L5 AND HYDROGENATION

=> d ibib abs l6 1-8

L6   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2007:362416  CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER:          148:121227
TITLE:                    Ruthenium catalyzed asymmetric hydrogenation
                          of α- and β-ketoesters in room temperature
                          ionic liquids using chiral P-Phos ligand
AUTHOR(S):                Xu, Lijin; Lam, Kim Hung; Ruan, Jiwu; Fan, Qinghua;
                          Chan, Albert S. C.
CORPORATE SOURCE:         Open Laboratory of Chirotechnology of the Institute of
                          Molecular Technology for Drug Discovery and Synthesis
                          and Department of Applied Biology and Chemical
                          Technology, The Hong Kong Polytechnic University, Hong
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Kong, Peop. Rep. China
SOURCE: ACS Symposium Series (2007), 950(Ionic Liquids in Organic Synthesis), 224-234
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:121227
AB Chiral dipyridyl phosphine ligand was found to be effective in the Ru-catalyzed asym. hydrogenation of α- and β-keto esters in room temperature ionic liqs. with high conversions and good to excellent enantioselectivities.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:37762 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 144:273900
TITLE: Multigram-scale asymmetric hydrogenation reactions using Ru-SYNPHOS and Ru-DIFLUORPHOS catalysts
AUTHOR(S): Jeulin, Severine; Champion, Nicolas; Dellis, Philippe; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels (UMR 7573 CNRS), Ecole Nationale Superieure de Chimie de Paris, Paris, 75231/05, Fr.
SOURCE: Synthesis (2005), (20), 3666-3671
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:273900
AB The detailed procedure for the synthesis of Ru-SYNPHOS and Ru-DIFLUORPHOS catalysts are described. These catalysts displayed high rates and are quite effective for the large-scale hydrogenation reactions of carbonyl compds., such as β-keto esters RCOCH2CO2Et (R = Me, ClCH2, F3C, Ph, PhCH2OCH2), acetylacetone and hydroxyacetone.
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1206596 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 144:107747
TITLE: Ruthenium catalyzed asymmetric hydrogenation of α- and β-keto esters in ionic liquids using chiral P-Phos ligand
AUTHOR(S): Lam, Kim Hung; Xu, Lijin; Feng, Lichun; Ruan, Jiwu; Fan, Qinghua; Chan, Albert S. C.
CORPORATE SOURCE: Open Laboratory of Chirotechnology of the Institute of Molecular Technology for Drug Discovery and Synthesis and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, Peop. Rep. China
SOURCE: Canadian Journal of Chemistry (2005), 83(6-7), 903-908
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:107747
AB Chiral dipyridylphosphine ligand was used in the Ru-catalyzed asym. hydrogenation of α- and β-keto esters in room temperature

ionic liqs. giving the corresponding α- and β-hydroxy esters with high conversions and good to excellent enantioselectivities. The catalyst was recycled by simple extraction and reused five times without loss of activity and enantioselectivity.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:626146 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 141:313992

TITLE: New developments in the synthesis of heterotopic atropisomeric diphosphines via diastereoselective aryl coupling reactions

AUTHOR(S): Madec, Jonathan; Michaud, Guillaume; Genet, Jean-Pierre; Marinetti, Angela

CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, UMR 7573, ENSCP 11, Paris, 75231, Fr.

SOURCE: Tetrahedron: Asymmetry (2004), 15(14), 2253-2261 CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:313992

AB The new heterotopic atropisomeric diphosphine (R)-5,6-benzo-2,2'-bis(diphenylphosphino)-4',5',6'-trimethylbiphenyl has been prepared The key step of this synthesis is a diastereoselective, intramol. aryl-aryl coupling reaction via oxidation of a suitable, chiral diarylcuprate. The catalytic properties of the diphosphine in ruthenium promoted hydrogenations of model substrates and in rhodium promoted 1,4-addns. of boronic acids to α,β-unsatd. ketones are fully comparable to those of reference ligands such as BINAP. This seems to indicate that C2-symmetry is not a structural prerequisite for atropisomeric chiral diphosphines to obtain high enantioselectivities in 1,4-addition reactions as well as in hydrogenation reactions.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:356392 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 141:71622

TITLE: Chiral biphenyl diphosphines for asymmetric catalysis: stereoelectronic design and industrial perspectives

AUTHOR(S): Jeulin, Severine; De Paule, Sebastien Duprat; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe

CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, Ecole Nationale Superieure de Chimie de Paris, Paris, 75231, Fr.

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(16), 5799-5804 CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:71622

GI

/ Structure 12 in file .gra /

AB Both enantiomers of the chiral diphosphines I (SYNPHOS) and II (DIFLUORPHOS) are prepared on multigram scales; the electronic and steric characteristics of I and II and of rhodium complexes derived from them are determined, compared with previous diphosphine catalysts, and correlated with their activities and enantioselectivities in the hydrogenation of ketones and olefins. I and II are prepared in five steps from 6-bromo-2,3-dihydro-1,4-benzodioxane and 5-bromo-2,2-difluorobenzodioxole, resp.; lithium-metal exchange and addition to a phosphoryl or phosphinyl chloride followed by oxidation to yield phosphine oxides, regioselective lithiation and iodination, Ullman coupling of the aryl iodides, resolution (either by acid-base resolution with di-O-benzoyl-tartaric acid or by chiral HPLC), and reduction of the phosphine oxides yields I and II in 38% and 33% overall yield, resp. The bite angles of I and II are compared to those of other common diphosphine ligands such as BINAP and MeO-BIPHEP. The structure of diastereomeric chlorohydridoruthenium complexes of (S)-II with Me acetoacetate is determined The C-O stretching frequencies of chloro(carbonyl)rhodium diphosphine complexes containing I, II, BINAP, and MeO-BIPHEP are determined as a measure of the electronic demands of the diphosphine ligands. β-Keto ester, α-keto ester, 1,3-diketone, ketone, and olefin substrates are hydrogenated in the presence of nonracemic I, II, BINAP, and MeO-BIPHEP and bis(η3-methallyl)(η4-1,5-cyclooctadienyl)ruthenium; the enantioselectivities are correlated with the steric and electronic properties of the ligands. The stereoelectronic features of the ligand and the substrate deeply influence the enantioselectivities obtained in asym. hydrogenation; whereas the steric and electronic factors for I (as in other diphosphines) correlate well, the bite angle of II does not correlate to its electronic effects in asym. hydrogenation reactions, leading to complementary hydrogenation selectivities for ligands I and II.

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:70307 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 140:253116
TITLE: Difluorphos, an electron-poor diphosphane: A good match between electronic and steric features
AUTHOR(S): Jeulin, Severine; Duprat de Paule, Sebastien; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, Ecole Nationale Superieure de Chimie de Paris, Paris, 75231, Fr.
SOURCE: Angewandte Chemie, International Edition (2004), 43(3), 320-325
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:253116
GI

/ Structure 13 in file .gra /

AB Both enantiomers of difluorphos I were synthesized and their stereoelectronic features were evaluated in theor. and exptl. studies. The unusual π acidity of I explains the excellent results obtained with it in ruthenium-mediated asym. hydrogenation of fluorinated β-functionalized ketones. These results are better than those obtained with other biphenyl-based diphosphines.
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:502611 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 121:102611
ORIGINAL REFERENCE NO.: 121:18339a,18342a
TITLE: purification and characterization of a novel carbonyl reductase isolated from Rhodococcus erythropolis
AUTHOR(S): Zelinski, Thomas; Peters, Joerg; Kula, Maria-Regina
CORPORATE SOURCE: Institut fuer Enzymtechnologie der Heinrich-Heine-Universitaet Duesseldorf, Forschungszentrum Juelich (KFA), Julich, 52404, Germany
SOURCE: Journal of Biotechnology (1994), 33(3), 283-92
CODEN: JBITD4; ISSN: 0168-1656
DOCUMENT TYPE: Journal
LANGUAGE: English
AB During growth on n-tetradecane a novel NADH-dependent carbonyl reductase is induced in the Gram-pos. bacterium Rhodococcus erythropolis (Peters, P., Zelinski, T. and Kula, M.R. (1992) Appl. microbiol. biotechnol. 38, 334-340). The enzyme has been purified to homogeneity using fractional pH precipitation, anion exchange chromatog. and affinity chromatog. The isoelec. point of the oxidoreductase is 4.4. The apparent mol. mass of the native enzyme is 161 kDa, that of the subunits 40 kDa as determined by SDS gel electrophoresis. A tetrameric structure of the carbonyl reductase is consistent with these results. Important biochem. data concerning the application of the reductase are: a broad pH-optimum, temperature optimum at 40° and stability at room temperature for more than 5 days. The oxidoreductase accepted as substrate aliphatic and aromatic ketones, keto esters (esters of keto carboxylic acids) and halogenated carbonyl compds. and reduced them to the corresponding hydroxyl compds. with (S)-configuration with more than 98% enantiomeric excess. The NAD+-dependent oxidation of primary alcs. was not catalyzed by the carbonyl reductase, whereas secondary alcs. and hydroxy acid esters were oxidized to the corresponding carbonyl compds. at about 10-fold slower reaction rates compared to the reduction

L6 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:603787 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 119:203787
ORIGINAL REFERENCE NO.: 119:36369a,36372a
TITLE: Stereodivergent synthesis of fluorinated threonine derivatives in high optical purity
AUTHOR(S): Shimizu, Makoto; Yokota, Tetsuya; Fujimori, Kouichi; Fujisawa, Tamotsu
CORPORATE SOURCE: Dep. Chem. Mater., Mie Univ., Tsu, 514, Japan
SOURCE: Tetrahedron: Asymmetry (1993), 4(5), 835-8
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:203787
AB Fluorinated 3-acetoxy-2-(methoxyimino)butyrates were resolved by lipase to

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     give the corresponding alcs. and the acetates in high optical purity.  The
     resolved alcs. were readily converted into mono-, di-, and
     trifluorothreonine and allothreonine derivs. by hydrogenation of
     the methoxyimino group.
http://www.cas.org/support/stngen/stndoc/properties.html

=> e "ethyl 4-bromo-3-oxobutanoate"/cn
E1            1      ETHYL 4-BROMO-3-METHYLTHIOPHENE-2-CARBOXYLATE/CN
E2            1      ETHYL 4-BROMO-3-NITROBENZOATE/CN
E3            1 --> ETHYL 4-BROMO-3-OXOBUTANOATE/CN
E4            1      ETHYL 4-BROMO-3-OXOBUTANOATE, COPPER COMPLEX/CN
E5            1      ETHYL 4-BROMO-3-OXOBUTYRATE/CN
E6            1      ETHYL 4-BROMO-3-OXOCYCLOHEXANECARBOXYLATE/CN
E7            1      ETHYL 4-BROMO-3-OXOHEPTANOATE/CN
E8            1      ETHYL 4-BROMO-3-OXOHEXANOATE/CN
E9            1      ETHYL 4-BROMO-3-OXONONANOATE/CN
E10           1      ETHYL 4-BROMO-3-OXOPENTANOATE/CN
E11           1      ETHYL 4-BROMO-3-OXOVALERATE/CN
E12           1      ETHYL 4-BROMO-3-PROPYLHEPTANOATE/CN

=> e "ethyl 4-bromo-3-hydroxybutanoate"/cn
E1            1      ETHYL 4-BROMO-3-ETHOXYCROTONATE/CN
E2            1      ETHYL 4-BROMO-3-HYDROXYBENZOATE/CN
E3            1 --> ETHYL 4-BROMO-3-HYDROXYBUTANOATE/CN
E4            1      ETHYL 4-BROMO-3-HYDROXYBUTYRATE/CN
E5            1      ETHYL 4-BROMO-3-HYDROXYCYCLOHEXANECARBOXYLATE/CN
E6            1      ETHYL 4-BROMO-3-HYDROXYPIPERIDINE-1-CARBOXYLATE/CN
E7            1      ETHYL 4-BROMO-3-METHOXY-2-PENTENOATE/CN
E8            1      ETHYL 4-BROMO-3-METHOXYCROTONATE/CN
E9            1      ETHYL 4-BROMO-3-METHOXYPHENOXYACETATE/CN
E10           1      ETHYL 4-BROMO-3-METHOXYTHIOFURAN-2-CARBOXYLATE/CN
E11           1      ETHYL 4-BROMO-3-METHOXYTHIOPHENE-2-CARBOXYLATE/CN
E12           1      ETHYL 4-BROMO-3-METHYL-2-BUTENOATE/CN

=> s e3
L7            1 "ETHYL 4-BROMO-3-HYDROXYBUTANOATE"/CN

=> d l7 ide

L7   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   32224-01-4  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Butyric acid, 4-bromo-3-hydroxy-, ethyl ester (7CI, 8CI)
OTHER NAMES:
CN   (±)-Ethyl 4-bromo-3-hydroxybutyrate
CN   4-Bromo-3-hydroxybutanoic acid ethyl ester
CN   Ethyl γ-bromo-β-hydroxybutyrate
CN   Ethyl 4-bromo-3-hydroxybutanoate
CN   Ethyl 4-bromo-3-hydroxybutyrate
DR   128052-98-2
MF   C6 H11 Br O3
LC   STN Files:   BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
        (*File contains numerically searchable property data)


/ Structure 14 in file .gra /
http://www.cas.org/legal/infopolicy.html

=> s l7
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L9 17 L7

=> d l9 ibib abs 1-17

L9 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:974948 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 149:268051
TITLE: Preparation of benzimidazole, benzothiazole and benzoxazole derivatives and their use as LTA4 hydrolase modulators
INVENTOR(S): Barchuk, William T.; Dunford, Paul J.; Edwards, James P.; Fourie, Anne M.; Karlsson, Lars; Quan, Joanne M.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 140pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20080194630	A1	20080814	US 2008-69943	20080214
WO 2008100564	A1	20080821	WO 2008-US1949	20080214

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2007-889851P P 20070214
OTHER SOURCE(S): MARPAT 149:268051
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I and related phenethylamine and phenoxyethylamine analogs are disclosed [X = NH, NMe, O, S; Y = CH2, O; R4 = H, OMe, Cl, F, Br, I, OH, NH2, CN, CF3, Me; R6 = H, F; R2, R3 = independently alk(en/yn)yl, SO2-alkyl, alkylheteroaryl; or NR2R3 = (un)substituted heterocyclyl]. Leukotriene A4 hydrolase (LTA4H) inhibitors of formula I, including their enantiomers, diastereomers, racemics, tautomers, hydrates, solvates or pharmaceutically acceptable salts, esters, or amides, compns. containing them, and their use for the treatment, prevention or inhibition of inflammation and/or conditions associated with inflammation are disclosed. For example, II was prepd, in 63% yield, by amination of 2-[4-(2-bromoethoxy)phenoxy]benzothiazole (preparation given) with 1-(piperidin-4-yl)pyrrolidin-2-one hydrochloride. II displayed a IC50 of 1 nM in a recombinant human LTA4 hydrolase assay.

L9 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:873237 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 147:277913
TITLE: Improved method and kit for automated resolving agents, especially amino acid derivatives, and solvents selection
INVENTOR(S): Vaidya, Niteen A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 29pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070185346	A1	20070809	US 2006-347532	20060203
WO 2007092264	A2	20070816	WO 2007-US2800	20070131
WO 2007092264	A3	20071129		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1981831	A2	20081022	EP 2007-763121	20070131
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: US 2006-347532 A2 20060203
WO 2007-US2800 W 20070131

AB The invention is related to a kit for improved identification of the optimal conditions for diastereomeric salt crystallization and the selection of the optimal resolving agents, especially amino acid derivs., and solvents, which include A. an array of containers wherein the array is a standard high throughput tray and the containers are a multiplicity of substantially identical containers or well plates each optionally sealed with a sealant or stoppers to avoid loss of chemical solvent; B. wherein each substantially identical container has a unique combination of resolving agent in each column and at least one suitable solvent in each row; and C. an instructional text to use said kit. The tray of 24, 48, 96 or more samples is examined simultaneously visually or by standard anal. techniques. Resolution of (±)-2-phenylpropionic acid was studied with both amines and acids as resolving agents. Strychnine in 96% ethanol was ideal system for (+)-isomer, while quinidine in 96% ethanol was the system of choice for (-)-isomer. Pyroglutamic acid in 70% isopropanol was ideal system for (+)-isomer, while malic acid in in 1-butanol was the system of choice for (-)-isomer.

L9 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1267800 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 146:242727
TITLE: Enantiomeric impurities in chiral synthons, catalysts, and auxiliaries: Part 3
AUTHOR(S): Huang, Ke; Breitbach, Zachary S.; Armstrong, Daniel W.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of Texas at Arlington, Arlington, TX, 76019, USA
SOURCE: Tetrahedron: Asymmetry (2006), 17(19), 2821-2832
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The enantiomeric excess of chiral reagents used in asym. syntheses directly affects the reaction selectivity and product purity. Eighty-four of the more recently available chiral compds. were evaluated to determine their actual enantiomeric composition These compds. are widely used in asym. syntheses as chiral synthons, catalysts, and auxiliaries. These include chiral alcs., amines, amino alcs., amides, carboxylic acids, epoxides, esters, ketones, and oxolanes among other classes of compds. All enantiomeric test results were categorized within five impurity levels (i.e., <0.01%, 0.01-0.1%, 0.1-1%, 1-10%, and >10%). The majority of the reagents tested have enantiomeric impurities over 0.01%, and two of them contain enantiomeric impurities exceeding the 10% level. The most effective enantioselective anal. method was a GC approach using a Chiraldex GTA chiral stationary phase (CSP). This method worked exceedingly well with chiral amines and alcs.
REFERENCE COUNT: 121 THERE ARE 121 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1240791 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 143:476533
TITLE: The method of making optically active ester derivatives and their acids from racemic esters
INVENTOR(S): Chung, Sun Ho; Hwang, Soon Ook
PATENT ASSIGNEE(S): Enzytech, Ltd., S. Korea
SOURCE: PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005111227	A1	20051124	WO 2005-KR1213	20050427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2005104481	A	20051103	KR 2004-29791	20040429
EP 1740714	A1	20070110	EP 2005-764804	20050427
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1946855	A	20070411	CN 2005-80013419	20050427
US 20080038802	A1	20080214	US 2006-587228	20061023
PRIORITY APPLN. INFO.:			KR 2004-29791 A	20040429
			WO 2005-KR1213 W	20050427

OTHER SOURCE(S): MARPAT 143:476533

AB The present invention relates to process for the preparing of optically active ester derivs. and their acid derivs. which are used intensively as important chiral intermediates from racemic β-hydroxybutyl ester derivs. In more detail, this invention relates to the process for preparing optically active β-hydroxybutyl ester derivs. and their acid derivs. by stereospecific hydrolysis of racemic β-hydroxybutyl ester derivs. using lipases or lipase-producing microorganisms in the aqueous phase or organic phase including aqueous solvent. The method of making optically active ester derivs. and their acid derivs. by hydrolysis of β-hydroxybutyl ester derivs. is easier and more economical than conventional methods and the products have high optical purity. Also, separation of ester derivs. from acid derivs. is easy after reaction. Thus, this method is a useful process on the industrial scale.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:120925 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 142:219285

TITLE: Preparation of benzimidazole, benzothiazole and benzoxazole derivatives and their use as LTA4 hydrolase modulators

INVENTOR(S): Axe, Frank U.; Bembenek, Scott D.; Butler, Christopher R.; Edwards, James P.; Fourie, Anne M.; Grice, Cheryl A.; Savall, Brad M.; Tays, Kevin L.; Wei, Jianmei

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 390 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012296	A1	20050210	WO 2004-US24050	20040727
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004261610	A1	20050210	AU 2004-261610	20040727
CA 2534212	A1	20050210	CA 2004-2534212	20040727
US 20050043378	A1	20050224	US 2004-900103	20040727
US 20050043379	A1	20050224	US 2004-900152	20040727
EP 1660491	A1	20060531	EP 2004-779219	20040727
EP 1660491	B1	20080806		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
BR 2004013072	A	20061003	BR 2004-13072	20040727
CN 1856490	A	20061101	CN 2004-80027906	20040727
JP 2007500703	T	20070118	JP 2006-521973	20040727
SG 129449	A1	20070226	SG 2007-691	20040727
SG 130192	A1	20070320	SG 2007-817	20040727
AT 403654	T	20080815	AT 2004-779219	20040727

AT 405562	T	20080915	AT 2004-779375		20040727
MX 2006PA01122	A	20060907	MX 2006-PA1122		20060127
KR 2006054408	A	20060522	KR 2006-702211		20060131
NO 2006000823	A	20060315	NO 2006-823		20060220
PRIORITY APPLN. INFO.:			US 2003-490710P	P	20030728
			WO 2004-US24050	W	20040727

OTHER SOURCE(S): CASREACT 142:219285; MARPAT 142:219285
GI

L9 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:55193 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 142:155558
TITLE: Cyanation method for producing 4-cyano-3-hydroxybutyric acid esters from their corresponding 4-leaving-group-substituted derivatives and cyanide salts
INVENTOR(S): Eckert, Markus; Rodefeld, Lars; Brackemeyer, Thomas; Dreisbach, Claus; Rampf, Florian; Schlummer, Bjoern
PATENT ASSIGNEE(S): Bayer Chemicals AG, Germany
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005005375	A1	20050120	WO 2004-EP7030	20040629
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10331211	A1	20050127	DE 2003-10331211	20030710
PRIORITY APPLN. INFO.:			DE 2003-10331211 A	20030710

OTHER SOURCE(S): CASREACT 142:155558; MARPAT 142:155558
AB 4-Cyano-3-hydroxybutyric acid esters (e.g., Et 4-cyano-3-hydroxybutyrate) are prepared by the cyanation-substitution reaction of 4-leaving-group-substituted-3-hydroxybutyric acid esters (e.g., Et 4-chloro-3-hydroxybutyrate) with a cyanide salt (e.g., sodium cyanide) in an organic solvent (formamide) in the presence of one or several other salts (sodium dihydrogenphosphate).
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:308406 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 140:321018
TITLE: Process for the preparation of a lower alkyl 4-cyano-3-hydroxybutyrate from 3-hydroxy-γ-butyrolactone
INVENTOR(S): Kwon, Taesoo; Gu, Chen; Yang, Soon-Ha
PATENT ASSIGNEE(S): SK Energy and Chemical Inc., USA

SOURCE: PCT Int. Appl., 11 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031131	A1	20040415	WO 2003-US30869	20030930
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2500668	A1	20040415	CA 2003-2500668	20030930
AU 2003272793	A1	20040423	AU 2003-272793	20030930
EP 1551796	A1	20050713	EP 2003-754994	20030930
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1688539	A	20051026	CN 2003-823536	20030930
JP 2006502201	T	20060119	JP 2004-541917	20030930
IN 2005DN01239	A	20070119	IN 2005-DN1239	20050330

PRIORITY APPLN. INFO.: US 2002-415672P P 20021003
WO 2003-US30869 W 20030930
OTHER SOURCE(S): CASREACT 140:321018
AB Alkyl 4-cyano-3-hydroxybutyrates are prepared by: (a) reacting 3-hydroxy-γ-butyrolactone using a haliding reagent in the presence of an acylating agent in a lower alkanol solvent so as to provide a reaction product comprising a lower alkyl 4-halo-3-hydroxybutyrate (halo = bromo, iodo); and (b) reacting the reaction product from step (a), without isolation or purification, with a source of cyanide ion (e.g., NaOH) in a reaction mixture having a pH of 7-11 to produce a lower alkyl 4-cyano-3-hydroxybutyrate (ACHB) with minimal byproduct formation.
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:935084 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 138:253757
TITLE: The enantioselectivity of reduction of ethyl 4-halo-3-oxobutanoate catalyzed by Geotrichum candidum depends on the cofactor
AUTHOR(S): Sundby, Eirik; De Zotti, Marta; Anthonsen, Thorleif
CORPORATE SOURCE: Department of Chemistry, Norwegian University of Science and Technology, Trondheim, N-7491, Norway
SOURCE: Journal of Molecular Catalysis B: Enzymatic (2003), 21(1-2), 63-66
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:253757
AB Enantioselective redns. of Et 3-oxobutanoates with fermenting cells or acetone treated cells of Geotrichum candidum gave 3-hydroxyesters with different ee and different predominant configurations depending on

reaction conditions. Et 4-bromo-3-oxobutanoate was reduced with APG4 and NADH to give predominantly Et (R)-4-bromo-3 hydroxybutanoate while the (S)-configuration was predominant when NADPH was the cofactor. Moreover, when the catalyst was heated before the reaction, the ee was increased indicating that the enzyme giving the (S)-alc. is more thermolabile than the other.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:268357 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 120:268357
ORIGINAL REFERENCE NO.: 120:47523a,47526a
TITLE: Manufacture of (S)-gamma-halogenated-beta-hydroxybutrylic acid esters for pharmaceutical synthesis
INVENTOR(S): Oonishi, Ikumasa; Shimaoka, Megumi; Kira, Ikuo; Nakazawa, Masakazu
PATENT ASSIGNEE(S): Ajinomoto KK, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06038776	A	19940215	JP 1993-85938	19930413
JP 3163338	B2	20010508		
US 5413921	A	19950509	US 1993-66239	19930525
PRIORITY APPLN. INFO.:			JP 1992-137111 A1	19920528

AB The title compds. are prepared by reducing γ-halogenated acetoacetates asym. by microorganisms such as Stemphylium, Alternaria, Corynespora, Preussia, Neurospora, Kabatiella, Gelasinospora, Neocosmospora, Sporormiella, Torulaspora, Pachysolen, and Sterigumatomyces. These compds. are starting materials for pharmaceutical synthesis.

L9 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:438920 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 113:38920
ORIGINAL REFERENCE NO.: 113:6617a,6620a
TITLE: Manufacture of L-carnitine chloride with lipase
INVENTOR(S): Horinaka, Akio
PATENT ASSIGNEE(S): Earth Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02027995	A	19900130	JP 1988-177373	19880715
PRIORITY APPLN. INFO.:			JP 1988-177373	19880715

AB The title compound (I), useful in treatment of heart diseases, is manufactured by transesterification of XCH2CH(OH)CH2Y (II, X = Cl, Br, I; Y = CN, alkoxycarbonyl) with lipase in the presence of fatty acid esters, separation of L-II,and conversion of them into I. II (X = Cl, Y = CN (III)) 4.78 and

9.88 g 2,2,2-trichloroethyl caproate were treated with lipase adsorbed on celite in ether at room temperature for 4 days and purified by silica gel column
chromatog. to give 2.29 g unreacted III, which was treated with 30% trimethylamine aqueous solution at 4° overnight to afford 0.83 g L-carnitinenitrile. Treatment of the nitrile (0.8 g) with concentrated HCl at 90° for 4 h gave 0.67 g I.

L9 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:178661 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 112:178661
ORIGINAL REFERENCE NO.: 112:30213a,30216a
TITLE: Preparation of 1-benzyl-4-hydroxy-2-pyrrolidinone as an intermediate for drugs and agrochemicals
INVENTOR(S): Kutsuki, Hidetoshi; Maemoto, Shunichi; Hasegawa, Junzo
PATENT ASSIGNEE(S): Kanegafuchi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01254658	A	19891011	JP 1988-83630	19880404
PRIORITY APPLN. INFO.:			JP 1988-83630	19880404

AB The title compound was prepared by treatment of 4-halo-3-hydroxybutyric esters with PhCH2NH2 (I), its salts, or their mixture ClCH2CH(OH)CH2CO2Et and II in EtOH were refluxed 50 h with Na2CO3 to give 63% I.

L9 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:157695 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 112:157695
ORIGINAL REFERENCE NO.: 112:26651a,26654a
TITLE: Preparation of optically active 4-halo-3-hydroxybutyric acid esters and carnitine
INVENTOR(S): Noyori, Ryoji; Kitamura, Masahito; Okuma, Takeshi; Kumobayashi, Hidenori
PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01211551	A	19890824	JP 1988-37032	19880219
JP 06078277	B	19941005		
EP 339764	A1	19891102	EP 1989-301585	19890217
EP 339764	B1	19920624		
R: CH, DE, FR, GB, IT, LI, NL				
US 4895979	A	19900123	US 1989-313007	19890221
PRIORITY APPLN. INFO.:			JP 1988-37032 A	19880219

OTHER SOURCE(S): CASREACT 112:157695; MARPAT 112:157695
GI

/ Structure 17 in file .gra /

AB XCH2CH(OH)CH2CO2R (I; R = lower alkyl; X = Cl, Br) are prepared by asym. hydrogenation of XCH2COCH2CO2R (II) in the presence of Ru2Cl4L2NEt3 (L = Q; R1 = H, Me, CMe3), Ru(OCOR2)2L (R2 = lower alkyl, CF3), or RuX2L at 70-150° and carnitine (III) is prepared by treatment of I with Me3N without isolation. A mixture of II (R = Et, X = Cl), EtOH, and RuBr2L [L = (-)-Q, R1 = H] was autoclaved under 100 kg/cm2 H at 100° for 10 min to give 97% (3R)-(+)-I (R = Et, X = Cl) with 97.2% e.e, vs. 47.0% and 67.0% e.e., resp., for a control using RuBr2L [L =(+)-Q, Q1 = H] at 19° for 16 h. A mixture of II (R = Me, X = Cl), MeOH, and Ru(OAc)2L [L = (-)-Q, R1 = H] was autoclaved under 100 kg/cm2 H at 100° for 15 min, after distillation out MeOH and addition of an aqueous Me3N solution, the reaction mixture was further stirred at 70° for 1.5 h and at 90° for 30 min to give 46% III.Cl.

L9 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 110:191289
ORIGINAL REFERENCE NO.: 110:31739a,31742a
TITLE: Enzymic manufacture of γ-substituted β-hydroxybutyrate esters as intermediates for carnitine synthesis
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo; Kato, Masaaki; Morikawa, Tadashi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		
PRIORITY APPLN. INFO.:			JP 1987-145587	19870611

AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ-substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which form two phases with H2O. Sporobolomyces salmonicolor IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ-chloroacetoacetate, NADPH, and AcOEt at 30° and pH 8 for 20 h under stirring to produce 92% Et γ-chloro-β-hydroxybutyrate, vs. 52% in the absence of AcOEt.

L9 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:32369 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 106:32369
ORIGINAL REFERENCE NO.: 106:5415a,5418a
TITLE: Asymmetric reduction of β-keto esters
INVENTOR(S): Ai, Kenzo
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61155354	A	19860715	JP 1984-281337	19841227

PRIORITY APPLN. INFO.: JP 1984-281337 19841227

AB R1COCH2CO2R2 (R1, R2 = alkyl, alkenyl, alkynyl, aryl, aralkyl, etc.) are asym. reduced in the presence of [R3NR5CHR4(CH2)mY]n (R3, R5 = H, amino-protecting group, R3R5N = heterocycle; R4 = CO2H, CH2OH; m = 0-3; Y = SH, OH, NH2, CO2H when n = 1; Y = S when n = 2) and C1-20 alcs., PhOH, benzyl alc. etc. Thus, LiBH4 was added to a solution of 1.21 mmol (R,R)-N,N'-dibenzoylcystine and 1.61 mmol Me3COH in THF, refluxed, cooled, 1.01 mmol PhCOCH2CO2Et added, and the mixture stirred at -30° to give 94% (R)-(+)-PhCH(OH)CH2CO2Et of 87% optical yield.

L9 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:50233 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 88:50233
ORIGINAL REFERENCE NO.: 88:7917a,7920a
TITLE: Studies on ketene and its derivatives. LXXXV. Reactions of 4-bromo-3-hydroxybutanoate and its acyl derivatives
AUTHOR(S): Kato, Tetsuzo; Kimura, Hitoshi
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1977), 25(10), 2692-6
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:50233

AB Acylation of Et 4-bromo-3-hydroxybutanoate with Ac2O, BzCl, diketene, and Ph isocyanate gave Et 3-acetoxy- (I), Et 3-benzoyloxy- (II), Et 3-acetoacetoxy- (III), and Et 3-(N-phenylcarbamoyloxy)-4-bromobutanoate (IV), resp. Treating I with NaOEt-EtOH gave Et 4-hydroxycrotonate (V) and Et 4-bromocrotonate (VI). II similarly gave VI and Et 4-benzoyloxycrotonate. III was converted to V, Et 4-acetoacetoxycrotonate, and 3-acetyl-4-ethoxycarbonylmethyltetrahydrofuran-2-one. Conversely IV under the same conditions gave Et 4-anilinocrotonate instead of the acyl-migrated product.

L9 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:61218 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 60:61218
ORIGINAL REFERENCE NO.: 60:10777g,10778b-d
TITLE: A new synthesis of carnitine
AUTHOR(S): D'Alo, F.; Masserini, A.
CORPORATE SOURCE: Lab. Ric. Vister, Como, Italy
SOURCE: Farmaco, Edizione Scientifica (1964), 19(1), 30-4
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:61218

AB A synthesis of carnitine [DL-β-hydroxy-γtrimethylaminobutyric acid betaine, (I)] without the use of alkaline cyanide was carried out, beginning with Et γ-bromo-acetoacetate (II). At 5-10°, 209 g. II in 3200 ml. EtOH was added slowly to a solution of 12.65 g. NaBH4 in

25 ml. H2O, the mixture stirred 4 hrs. at 30°, excess NaBH4 decomposed with HOAc, the solution evaporated to dryness, taken up in saturated NaCl, and extracted with Et2O, and the extract dried (Na2SO4), evaporated, and distilled in vacuo to give 50% Et γ-bromo-β-hydroxybutyrate (III), b0.8 93-5°. III (21.1 g.) in 36 g. 33% Me3N in H2O was kept 12 hrs. and evaporated in vacuo, the residue in 200 ml. 10% HCl refluxed 3 hrs., the mixture evaporated to dryness in vacuo, and the residue taken up in 60 ml. absolute EtOH; the mixture of carnitine-HBr and -HCl which crystallized was dissolved in H2O, the solution passed through a column of 300 g. of Amberlite IR-45, and the column washed to a volume of 3 l. The aqueous solution was evaporated to 300 ml. in vacuo and stirred with 30 ml. Amberlite IRA-400 to remove traces of halide ion. After filtration the solution was evaporated to dryness in vacuo at 35°, the residue dissolved in 100 ml. of absolute EtOH, and the solution cooled in brine-ice mixture and precipitated with 250 ml. Me2CO to give 30% I. In the same manner, γ-amino-β-hydroxybutyric acid (IV), m. 215.5-17.5°, was prepared from III, with 33 ml. concentrated NH4OH instead of Me3N. The HCl solution was extracted with Et2O before refluxing; exchange was carried out on Amberlite IR-45 only, and the halide-free residue was recrystd. from 1:1 EtOH-H2O. The use of IV as an intermediate in the synthesis of I was not recommended because of the poor yield. Carter and Bhattacharya, CA 49, 3819f.

L9 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	1930:44129 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER:	24:44129
ORIGINAL REFERENCE NO.:	24:4759a-d
TITLE:	Oxidation of unsaturated compounds. II. Preparation and configuration of the 3-halogeno derivatives of crotonic acid
AUTHOR(S):	Braun, Geza
SOURCE:	Journal of the American Chemical Society (1930), 52, 3167-76 CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE:	Journal
LANGUAGE:	Unavailable
OTHER SOURCE(S):	CASREACT 24:44129

AB cf. C. A. 23, 817. ClCH2CH(OH)CH2CN (I) results in 65% yield by heating 500 g. epichlorohydrin and 145 g. HCN in dilute NaOH at 75-85° for 90 h. or in 25% yield (based on NaCN used) by adding 100 g. NaCN to 300 g. dichlorohydrin in 500 cc. H2O during 20 min. at 60° and then gradually raising the temperature to 100° during 2 h. I (500 g.) in 260 cc. absolute EtOH and 500 cc. dry Et2O, saturated with HCl at -15° during 6-8 h., the Et2O and excess HCl removed, the residue dissolved in 1 l. H2O and kept at 45-50° for 0.5 h., gives 81% of ClCH2CH(OH)CH3CO3Et, dehydrated by P2O6 to 62.5% of a mixture of about 80% of ClCH3CH:CHCO3Et and 20% of ClCH:CHCH2CO2Et. Saponification of the ester is best carried out with Ba(OH)2 below 0°; 100 g. of the ester gives 40 g. ClCH2CH:CHCO2H (II), m. 83°, and 18 g. of an acid, probably ClCH:CHCH2CO3H, m. 2-5° (recrystn. gives 10 g. of the acid, m. 10°). Reduction of the 3,3,3-tri-Cl derivative with Zn in EtOH-AcOH gives 80-85% of the 3,3-di-Cl derivative (III). Details are given for the preparation of dibromohydrin in 54% yield from C3H3(OH)3, Br and red P; with KCN there results 16.5% of 2-hydroxy-3-bromobutyronitrile, b2 117-8°; hydrolysis gives 70% of

Et 2-hydroxy-3-bromobutyrate, b3, 94-6°; P2O6 gives 28.5% of Et 3-bromocrotonate, b2 80-2°; Ba(OH)3 below 0° 50% of 3-bromocrotonic acid, m. 74°; the saturated aqueous solution contains at room temperature about 3% of acid. The Et ester of II and NaI in Me2CO give Et 3-iodocrotonate b2 90-2° (slight decomposition); it is lactrymatory and causes blisters on the skin; the free acid, yellow, m. 108-8.5° (86% yield), II is catalytically reduced to crotonic acid in about 95% yield; this indicates that II belongs to the crotonic acid series and has the trans-configuration according to Auwers. The reduction of the 3-Br acid proceeds much more slowly and the 3-I acid could not be reduced at all under the conditions used for II. Since the Cl and Br acids can be converted into the I acid, all 3 have the trans-configuration. II is an intermediate product in the reduction of III to crotonic acid.

http://www.cas.org/support/stngen/stndoc/properties.html

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=> e "ethyl 4,4,4-tribromo-3-hydroxybutanoate"/cn
E1            1     ETHYL 4,4'-DICHLOROBENZILATE/CN
E2            1     ETHYL 4,4'-DIHYDROXYDICOUMARINYL-3,3'-ACETATE/CN
E3            0 --> ETHYL 4,4,4-TRIBROMO-3-HYDROXYBUTANOATE/CN
E4            1     ETHYL 4,4,4-TRICHLORO-1-BUTENYL CARBONATE/CN
E5            1     ETHYL 4,4,4-TRICHLORO-1-TRIMETHYLSILYLBUTYL CARBONATE/CN
E6            1     ETHYL 4,4,4-TRICHLORO-2-BUTENOATE/CN
E7            1     ETHYL 4,4,4-TRICHLORO-2-CYANO-2-BUTENOATE/CN
E8            1     ETHYL 4,4,4-TRICHLORO-2-CYANOCROTONATE/CN
E9            1     ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
E10           1     ETHYL 4,4,4-TRICHLORO-3-OXOBUTANOATE/CN
E11           1     ETHYL 4,4,4-TRICHLOROACETOACETATE/CN
E12           1     ETHYL 4,4,4-TRICHLOROBUTANOATE/CN

=> e "ethyl 4,4-dibromo-3-hydroxybutanoate"/cn
E1            1     ETHYL 4,4-DIBROMO-2,2-DIETHYL-3-OXOPENTANOATE/CN
E2            1     ETHYL 4,4-DIBROMO-2,2-DIMETHYL-3-OXOBUTANOATE/CN
E3            0 --> ETHYL 4,4-DIBROMO-3-HYDROXYBUTANOATE/CN
E4            1     ETHYL 4,4-DIBROMOACETOACETATE/CN
E5            1     ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
                    ARBOXYLATE/CN
E6            1     ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E7            1     ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E8            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E9            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E10           1     ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E11           1     ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E12           1     ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN

=> s e2
L10           1 "ETHYL 4,4-DIBROMO-2,2-DIMETHYL-3-OXOBUTANOATE"/CN

=> d l10 ide

L10  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   151556-85-3  REGISTRY
ED   Entered STN:  03 Dec 1993
CN   Butanoic acid, 4,4-dibromo-2,2-dimethyl-3-oxo-, ethyl ester  (CA INDEX
     NAME)
OTHER NAMES:
CN   Ethyl 4,4-dibromo-2,2-dimethyl-3-oxobutanoate
MF   C8 H12 Br2 O3
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT, CHEMINFORMRX
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http://www.cas.org/support/stngen/stndoc/properties.html

```
=> e "methyl 4,4,4-trifluoro-3-hydroxybutanoate"/cn
E1            1      METHYL 4,4,4-TRIFLUORO-3-AMINO-2-BUTENOATE/CN
E2            1      METHYL 4,4,4-TRIFLUORO-3-HYDROXY-3-(2-MERCAPTO-1,3-THIAZOL-5
                     -YL)BUTANOATE/CN
E3            1 --> METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE/CN
E4            1      METHYL 4,4,4-TRIFLUORO-3-METHOXYBUTANOATE/CN
E5            1      METHYL 4,4,4-TRIFLUORO-3-METHYLTHIOBUTANOATE/CN
E6            1      METHYL 4,4,4-TRIFLUORO-3-OXOBUTANOATE/CN
E7            1      METHYL 4,4,4-TRIFLUOROACETOACETATE/CN
E8            1      METHYL 4,4,4-TRIFLUOROACETYLACETONATE/CN
E9            1      METHYL 4,4,4-TRIFLUOROBUTYNOATE/CN
E10           1      METHYL 4,4,4-TRIFLUOROBUTYRATE/CN
E11           1      METHYL 4,4,4-TRINITROBUTYRATE/CN
E12           1      METHYL 4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-HEPTADECAFLUOR
                     O-2-IODO-2-METHYLUNDECANOATE/CN

=> s e3
L1            1 "METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE"/CN

=> d l1 ide

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   475467-53-9  REGISTRY
ED   Entered STN:  09 Dec 2002
CN   Butanoic acid, 4,4,4-trifluoro-3-hydroxy-, methyl ester  (CA INDEX NAME)
OTHER NAMES:
CN   Methyl 4,4,4-trifluoro-3-hydroxybutanoate
MF   C5 H7 F3 O3
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT, USPAT2


/ Structure 19 in file .gra /


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> e "methyl 4,4,4-tribromo-3-hydroxybutanoate"/cn
E1            1      METHYL 4,4'-DIMETHOXYBENZILATE/CN
E2            1      METHYL 4,4'-DITHIODIBUTYRATE/CN
E3            0 --> METHYL 4,4,4-TRIBROMO-3-HYDROXYBUTANOATE/CN
E4            1      METHYL 4,4,4-TRICHLORO-3-METHYLBUTANOATE/CN
E5            1      METHYL 4,4,4-TRICHLOROBUTANOATE/CN
E6            1      METHYL 4,4,4-TRICHLOROBUTYRATE/CN
E7            1      METHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN
E8            1      METHYL 4,4,4-TRIFLUORO-3-((B-HYDROXYETHYL)AMINO)-3-(TRI
                     FLUOROMETHYL)BUTYRATE/CN
E9            1      METHYL 4,4,4-TRIFLUORO-3-(TRIFLUOROMETHYL)CROTONATE/CN
E10           1      METHYL 4,4,4-TRIFLUORO-3-AMINO-2-BUTENOATE/CN
E11           1      METHYL 4,4,4-TRIFLUORO-3-HYDROXY-3-(2-MERCAPTO-1,3-THIAZOL-5
                     -YL)BUTANOATE/CN
E12           1      METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE/CN

=> e "methyl 4,4,4-trichloro-3-hydroxybutanoate"/cn
E1            1      METHYL 4,4'-DIMETHOXYBENZILATE/CN
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E2            1     METHYL 4,4'-DITHIODIBUTYRATE/CN
E3            0 --> METHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
E4            1     METHYL 4,4,4-TRICHLORO-3-METHYLBUTANOATE/CN
E5            1     METHYL 4,4,4-TRICHLOROBUTANOATE/CN
E6            1     METHYL 4,4,4-TRICHLOROBUTYRATE/CN
E7            1     METHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN
E8            1     METHYL 4,4,4-TRIFLUORO-3-((B-HYDROXYETHYL)AMINO)-3-(TRI
                    FLUOROMETHYL)BUTYRATE/CN
E9            1     METHYL 4,4,4-TRIFLUORO-3-(TRIFLUOROMETHYL)CROTONATE/CN
E10           1     METHYL 4,4,4-TRIFLUORO-3-AMINO-2-BUTENOATE/CN
E11           1     METHYL 4,4,4-TRIFLUORO-3-HYDROXY-3-(2-MERCAPTO-1,3-THIAZOL-5
                    -YL)BUTANOATE/CN
E12           1     METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE/CN

=> e "ethyl 4,4,4-trichloro-3-hydroxybutanoate"/cn
E1            1     ETHYL 4,4,4-TRICHLORO-2-CYANO-2-BUTENOATE/CN
E2            1     ETHYL 4,4,4-TRICHLORO-2-CYANOCROTONATE/CN
E3            1 --> ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
E4            1     ETHYL 4,4,4-TRICHLORO-3-OXOBUTANOATE/CN
E5            1     ETHYL 4,4,4-TRICHLOROACETOACETATE/CN
E6            1     ETHYL 4,4,4-TRICHLOROBUTANOATE/CN
E7            1     ETHYL 4,4,4-TRICHLOROBUTENOATE/CN
E8            1     ETHYL 4,4,4-TRICHLOROBUTYRATE/CN
E9            1     ETHYL 4,4,4-TRIFLUORO-2-((2-HYDROXYETHYL)THIO)-3-OXOBUTANOAT
                    E/CN
E10           1     ETHYL 4,4,4-TRIFLUORO-2-BUTENOATE/CN
E11           1     ETHYL 4,4,4-TRIFLUORO-2-BUTYNECARBOXYLATE/CN
E12           1     ETHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN

=> s e3
L2            1 "ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE"/CN

=> d l2 ide

L2   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   19486-93-2  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Butyric acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN   Ethyl 4,4,4-trichloro-3-hydroxybutanoate
MF   C6 H9 Cl3 O3
LC   STN Files:   BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)

L3   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2002:886005  CAPLUS <<LOGINID::20081229>>
DN   137:369737
TI   Stereoselective hydrogen-transfer process and chiral ruthenium-diamine
     complex catalyst for producing optically active β-hydroxycarboxylate
     esters from β-ketocarboxylate esters and hydrogen donors
IN   Tada, Kenichi; Miura, Takashi
PA   Takasago International Corporation, Japan
SO   Eur. Pat. Appl., 9 pp.
     CODEN: EPXXDW
DT   Patent
LA   English
FAN.CNT 13
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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PI   EP 1258470          A2    20021120    EP 2002-291172         20020510
     EP 1258470          A3    20030813
     EP 1258470          B1    20050817
        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2003034665       A     20030207    JP 2002-82865          20020325
     JP 4015450          B2    20071128
     ES 2247280          T3    20060301    ES 2002-291172         20020510
     US 20030004362      A1    20030102    US 2002-142983         20020513
     US 6723871          B2    20040420
PRAI JP 2001-150012      A     20010518
     JP 2002-82865       A     20020325
OS   CASREACT 137:369737; MARPAT 137:369737
RE.CNT  2     THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
http://www.cas.org/support/stngen/stndoc/properties.html

=> e "ethyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1            1     ETHYL 4,4-DIBROMOACETOACETATE/CN
E2            1     ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
                    ARBOXYLATE/CN
E3            0 --> ETHYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1     ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5            1     ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8            1     ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9            1     ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10           1     ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11           1     ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12           1     ETHYL 4,4-DIETHOXYACETOACETATE/CN

=> s e1
L1            1 "ETHYL 4,4-DIBROMOACETOACETATE"/CN

=> d l1 ide

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   73817-88-6  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4-dibromo-3-oxo-, ethyl ester  (CA INDEX NAME)
OTHER NAMES:
CN   Ethyl 4,4-dibromoacetoacetate
MF   C6 H8 Br2 O3
LC   STN Files:   CA, CAPLUS, CASREACT, USPATFULL
 http://www.cas.org/legal/infopolicy.html

=> s l1
L2            2 L1

=> d l2 ibib abs 1-2

L2   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2003:49611  CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER:          138:237855
TITLE:                    Nonselective Bromination-Selective Debromination
                          Strategy: Selective Bromination of Unsymmetrical
                          Ketones on Singly Activated Carbon against Doubly
                          Activated Carbon
AUTHOR(S):                Choi, Han Young; Chi, Dae Yoon
```

CORPORATE SOURCE: Department of Chemistry, Inha University, Inchon, 402-751, S. Korea
SOURCE: Organic Letters (2003), 5(4), 411-414
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:237855

AB A new synthetic method for the preparation of α-bromo ketones that are brominated in the less activated terminal position of unsym. ketones is reported. Brominations for short reaction times (kinetically controlled) provided internally brominated compds. as the major product. However, brominations for longer reaction times (thermodynamically controlled) gave more of the terminally brominated compound through the reversible reaction by Br2 and produced hydrogen bromide. Several compds. brominated at the terminal position were successfully prepared through the new synthetic route.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:416984 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 93:16984
ORIGINAL REFERENCE NO.: 93:2787a,2790a
TITLE: Carbonylic halides as activators for phototropic compositions
INVENTOR(S): Reardon, Edward Joseph, Jr.; Lipson, Melvin A.
PATENT ASSIGNEE(S): Dynachem Corp., USA
SOURCE: Eur. Pat. Appl., 77 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 5379	A2	19791114	EP 1979-300795	19790509
EP 5379	A3	19791128		
EP 5379	B1	19811223		
EP 5379	B2	19860604		
R: BE, CH, DE, FR, GB, NL, SE				
CA 1153610	A1	19830913	CA 1979-326324	19790425
AU 7946767	A	19791115	AU 1979-46767	19790504
AU 523499	B2	19820729		
JP 54147829	A	19791119	JP 1979-56221	19790508
JP 63052368	B	19881018		
US 4552830	A	19851112	US 1983-555444	19831125
PRIORITY APPLN. INFO.:			US 1978-904144	19780509
			US 1980-195168 A2	19801008
			US 1981-317954 A1	19811103

OTHER SOURCE(S): MARPAT 93:16984

AB Compns., which are useful in the production of resists for use in the electronics industry to manufacture printed circuits, are composed of a polymerizable, curable, or crosslinkable component, a photoinitiator, a color former capable of changing color on contact with a suitable activator, and a latent activator containing an organic halide. The organic halide is a carbonyl compound, such as an aliphatic or cycloaliph. ketone or an ester or amide of a decarboxylic acid. A typical composition for the production of a dry

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     resist material contains a methacrylic acid-styrene (25:75) copolymer
     57.0, trimethylolpropane triacrylate 24.0, tetraethylene glycol diacrylate
     12.2, benzophenone 4.0, 4,4'-bis(dimethylamino)benzophenone 0.6,
     2-anilino-3-methoxy-6-diethylaminofluoran 0.3, di-Et iodomalonate 1.5,
     benzotriazole 0.4, and MeCOEt 160.0 parts kg weight  A dry resist using this
     composition is used to produce high quality printed circuit boards.
http://www.cas.org/support/stngen/stndoc/properties.html

=> e "ethyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1            1     ETHYL 4,4-DIBROMOACETOACETATE/CN
E2            1     ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
                    ARBOXYLATE/CN
E3            0 --> ETHYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1     ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5            1     ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8            1     ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9            1     ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10           1     ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11           1     ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12           1     ETHYL 4,4-DIETHOXYACETOACETATE/CN

=> e "methyl 4,4-dichloro-3-hydroxy-butanoate"/cn
E1            1     METHYL 4,4-DICHLORO-2-IODOBUTYRATE/CN
E2            1     METHYL 4,4-DICHLORO-2-OXO-3-BUTENOATE/CN
E3            0 --> METHYL 4,4-DICHLORO-3-HYDROXY-BUTANOATE/CN
E4            1     METHYL 4,4-DICHLOROACETOACETATE/CN
E5            1     METHYL 4,4-DICHLOROBUTANOATE/CN
E6            1     METHYL 4,4-DICHLOROBUTYRATE/CN
E7            1     METHYL 4,4-DICYANOBUTYRATE/CN
E8            1     METHYL 4,4-DIETHOXY-1-CYCLOBUTENECARBOXYLATE/CN
E9            1     METHYL 4,4-DIETHOXYBUT-2-YNOATE/CN
E10           1     METHYL 4,4-DIETHOXYCROTONATE/CN
E11           1     METHYL 4,4-DIFERROCENYL PENTANOATE/CN
E12           1     METHYL 4,4-DIFLUORO-2-HEXYNOATE/CN

=> s e2
L3            1 "METHYL 4,4-DICHLORO-2-OXO-3-BUTENOATE"/CN

=> d l3 ide

L3   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   36610-68-1  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   3-Butenoic acid, 4,4-difluoro-2-oxo-, methyl ester  (CA INDEX NAME)
OTHER NAMES:
CN   Methyl 4,4-dichloro-2-oxo-3-butenoate
MF   C5 H4 F2 O3
LC   STN Files:   CA, CAPLUS


/ Structure 22 in file .gra /


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

             1 REFERENCES IN FILE CA (1907 TO DATE)
             1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
http://www.cas.org/support/stngen/stndoc/properties.html
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```
=> e "t-butyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1            1      T-BUTYL/CN
E2            1      T-BUTYL 3A-(5-NORBORNENE-2-CARBONYLOXY)-5B-CHOLAN
                     -24-OATE-2-HYDROXYETHYL 5-NORBORNENE-2-CARBOXYLATE-MALEIC AN
                     HYDRIDE COPOLYMER/CN
E3            0 --> T-BUTYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1      T-BUTYL 6-TRIFLUOROMETHYL-3-(4-PYRIDINYLAMINO)INDOLE-2-CARBO
                     XYLATE/CN
E5            1      T-BUTYL ACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYLATE-
                     BUTYL METHACRYLATE-METHYL METHACRYLATE-METHACRYLIC ACID-DI-T
                     -BUTYL MALEATE COPOLYMER/CN
E6            1      T-BUTYL ACRYLATE-P-HYDROXYSTYRENE COPOLYMER/CN
E7            1      T-BUTYL ETHYL KETONE/CN
E8            1      T-BUTYL HYDROPEROXIDE/CN
E9            1      T-BUTYL IODIDE/CN
E10           1      T-BUTYL METHACRYLATE-1,3-BUTYLENE GLYCOL DIMETHACRYLATE COPO
                     LYMER/CN
E11           1      T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYL
                     ATE-2-HYDROXYETHYL METHACRYLATE COPOLYMER/CN
E12           1      T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYL
                     ATE-METHACRYLIC ACID COPOLYMER/CN

=> e "propyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1            1      PROPYL 4'-PENTANOYLOXYBIPHENYL-4-CARBOXYLATE/CN
E2            1      PROPYL 4,4-BIS(4-HYDROXYPHENYL)PENTANOATE/CN
E3            0 --> PROPYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1      PROPYL 4,5-EPOXY-2-HEXENOATE/CN
E5            1      PROPYL 4,6-DIHYDROXY-1,2,3,4-TETRAHYDROISOQUINOLINECARBOXYLA
                     TE/CN
E6            1      PROPYL 4,6-DIHYDROXY-2-METHYL-1,2,3,4-TETRAHYDROISOQUINOLINE
                     CARBOXYLATE/CN
E7            1      PROPYL 4,8-DIMETHYL-3,4-EPOXYNONANOATE/CN
E8            1      PROPYL 4,8-DIMETHYLNONANOATE/CN
E9            1      PROPYL 4-((2-HYDROXYBENZYL)AMINO)BENZOATE/CN
E10           1      PROPYL 4-((7-(2-FLUORO-4-(METHYLSULFONYL)PHENYL)-6,7-DIHYDRO
                     -5H-PYRROLO(2,3-D)PYRIMIDIN-4-YL)OXY)-1-PIPERIDINECARBOXYLAT
                     E/CN
E11           1      PROPYL 4-((AMINOSULFONYL)OXY)BENZOATE/CN
E12           1      PROPYL 4-(2-((TERT-BUTYLDIMETHYLSILYL)OXY)ETHYL)-3-FLUOROBEN
                     ZOATE/CN

=> e "4,4-dichloro-3-hydroxybutanoate'/cn
MISMATCHED QUOTE IN EXPAND TERM
Quotation marks (or apostrophes) must be used in pairs,
one before and one after the expression you are setting
off or masking.

=> e "4,4-dichloro-3-hydroxybutanoate"/cn
E1            1      4,4-DICHLORO-3-BUTENOYL CHLORIDE/CN
E2            1      4,4-DICHLORO-3-HEXANONE/CN
E3            0 --> 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1      4,4-DICHLORO-3-METHYL-5-PYRAZOLONE/CN
E5            1      4,4-DICHLORO-3-OXOBUTANOIC ACID/CN
E6            1      4,4-DICHLORO-3-PHENYL-2-CYCLOBUTEN-1-ONE/CN
E7            1      4,4-DICHLORO-3-PHENYL-2-CYCLOBUTENONE/CN
E8            1      4,4-DICHLORO-3-PHENYL-3-BUTEN-2-ONE/CN
E9            1      4,4-DICHLORO-4-SILA-1-DECENE/CN
E10           1      4,4-DICHLORO-4-SILA-1-DOCOSENE/CN
E11           1      4,4-DICHLORO-5,5,5-TRIFLUORO-2-METHYLPENTANOYL CHLORIDE/CN
E12           1      4,4-DICHLORO-5,5,5-TRIFLUOROPENTANOYL BROMIDE/CN
```

```
=> e "phenyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1            1      PHENYL 4,4-BIS(4-HYDROXYPHENYL)PENTANOATE HOMOPOLYMER/CN
E2            1      PHENYL 4,4-DICHLORO-1-BUTANESULFONATE/CN
E3            0 --> PHENYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1      PHENYL 4,5-DICHLOROISOTHIAZOLE-3-CARBOXYLATE/CN
E5            1      PHENYL 4,5-DIMETHYLSALICYLATE/CN
E6            1      PHENYL 4,5-EPOXY-2-HEXENOATE/CN
E7            1      PHENYL 4,6-DI-O-ACETYL-2,3-DIDEOXY-A-D-ERYTHRO-HEX-2-E
                     NOPYRANOSIDE/CN
E8            1      PHENYL 4,6-DI-O-ACETYL-2,3-DIDEOXY-B-D-ERYTHRO-HEX-2-EN
                     OPYRANOSIDE/CN
E9            1      PHENYL 4,6-O-BENZYLIDENE-B-D-GLUCOPYRANOSIDE/CN
E10           1      PHENYL 4,6-O-BENZYLIDENE-1-SELENO-B-D-GLUCOPYRANOSIDE/C
                     N
E11           1      PHENYL 4,6-O-BENZYLIDENE-2-DEOXY-2-PHTHALIMIDO-1-THIO-B
                     -D-GLUCOPYRANOSIDE/CN
E12           1      PHENYL 4-((((1R)-1-METHYL-2-((3-METHYLPHENYL)AMINO)-2-OXOETHY
                     L)OXY)BENZOATE/CN

=> e "isopropyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1            1      ISOPROPYL 4,4,4-TRIFLUOROACETOACETATE/CN
E2            1      ISOPROPYL 4,4,4-TRIFLUOROBUTYRATE/CN
E3            0 --> ISOPROPYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1      ISOPROPYL 4,4-DIETHOXYACETOACETATE/CN
E5            1      ISOPROPYL 4,5-DICHLOROPYRIDINE-2-CARBOXYLATE/CN
E6            1      ISOPROPYL 4,5-EPOXY-2-HEXENOATE/CN
E7            1      ISOPROPYL 4,6-DIHYDROXY-2-METHYL-1,2,3,4-TETRAHYDROISOQUINOL
                     INECARBOXYLATE/CN
E8            1      ISOPROPYL 4,6-DIMETHOXYPYRIMIDINE-2-CARBOXYLATE/CN
E9            1      ISOPROPYL 4-(((((2,4-DIMETHOXYPHENYL)AMINO)CARBONYL)OXY)METH
                     YL)PIPERIDINE-1-CARBOXYLATE/CN
E10           1      ISOPROPYL 4-((((5-TERT-BUTYL-2,3-DIHYDRO-1H-INDEN-1-YL)AMINO
                     )CARBONYL)AMINO)-1H-INDAZOLE-1-CARBOXYLATE/CN
E11           1      ISOPROPYL 4-((1-(1-(4-CHLOROPHENYL)CYCLOBUTYL)-3-METHYLBUTYL
                     )AMINO)BUTANOATE/CN
E12           1      ISOPROPYL 4-((4-CHLOROBENZOYL)AMINO)-2-(METHYLTHIO)-1-PHENYL
                     -1H-IMIDAZOLE-5-CARBOXYLATE/CN

=> e "ethyl 4,4-dichloro-3-hydroxybutyrate"/cn
E1            1      ETHYL 4,4-DIBROMOACETOACETATE/CN
E2            1      ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
                     ARBOXYLATE/CN
E3            0 --> ETHYL 4,4-DICHLORO-3-HYDROXYBUTYRATE/CN
E4            1      ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5            1      ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6            1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7            1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8            1      ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9            1      ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10           1      ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11           1      ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12           1      ETHYL 4,4-DIETHOXYACETOACETATE/CN
L5   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   1982:199025  CAPLUS <<LOGINID::20081229>>
DN   96:199025
OREF 96:32807a,32810a
TI   Alkoxyethynyl ketones
AU   Himbert, G.; Henn, L.
CS   Fachbereich Chem., Kaiserslautern, D-6750, Fed. Rep. Ger.
SO   Organic Preparations and Procedures International (1982), 14(3), 189-94
     CODEN: OPPIAK; ISSN: 0030-4948
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DT   Journal
LA   English
OS   CASREACT 96:199025

http://www.cas.org/support/stngen/stndoc/properties.html

=> s l5
L6            1 L4

=> d l6 all

L6   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   81711-50-4  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4-dichloro-3-oxo-, methyl ester  (CA INDEX NAME)
OTHER NAMES:
CN   Methyl 4,4-dichloroacetoacetate
MF   C5 H6 Cl2 O3
LC   STN Files:   CA, CAPLUS, CASREACT
DT.CA  CAplus document type:  Journal
RL.NP  Roles from non-patents:  PREP (Preparation)

=> s e4
L7            1 "ETHYL 4,4-DIFLUORO-3-OXOBUTANOATE"/CN

=> d l7 ide

L7   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   352-24-9  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4-difluoro-3-oxo-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Acetoacetic acid, 4,4-difluoro-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN   4,4-Difluoro-3-oxobutanoic acid ethyl ester
CN   Ethyl 4,4-difluoro-3-oxobutanoate
CN   Ethyl 4,4-difluoroacetoacetate
MF   C6 H8 F2 O3
CI   COM
LC   STN Files:   BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX,
       CHEMLIST, CSCHEM, TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:   EINECS**, NDSL**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)

http://www.cas.org/support/stngen/stndoc/properties.html

=> e "ethyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1            1      ETHYL 4,4-DIBROMOACETOACETATE/CN
E2            1      ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
                     ARBOXYLATE/CN
E3            0 --> ETHYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4            1      ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5            1      ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6            1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7            1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8            1      ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9            1      ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10           1      ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11           1      ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12           1      ETHYL 4,4-DIETHOXYACETOACETATE/CN
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=> s e4
L8            1 "ETHYL 4,4-DICHLORO-3-OXOBUTANOATE"/CN

=> d 18 ide

L8   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   6082-74-2  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4-dichloro-3-oxo-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Acetoacetic acid, 4,4-dichloro-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN   Ethyl 4,4-dichloro-3-oxobutanoate
MF   C6 H8 Cl2 O3
LC   STN Files:   BEILSTEIN*, CA, CAPLUS
         (*File contains numerically searchable property data)

=> e "ethyl 4,4-dibromo-3-hydroxybutanote'/cn
MISMATCHED QUOTE IN EXPAND TERM
Quotation marks (or apostrophes) must be used in pairs,
one before and one after the expression you are setting
off or masking.

=> e "ethyl 4,4-dibromo-3-hydroxybutanoate"/cn
E1            1     ETHYL 4,4-DIBROMO-2,2-DIETHYL-3-OXOPENTANOATE/CN
E2            1     ETHYL 4,4-DIBROMO-2,2-DIMETHYL-3-OXOBUTANOATE/CN
E3            0 --> ETHYL 4,4-DIBROMO-3-HYDROXYBUTANOATE/CN
E4            1     ETHYL 4,4-DIBROMOACETOACETATE/CN
E5            1     ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
                    ARBOXYLATE/CN
E6            1     ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E7            1     ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E8            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E9            1     ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E10           1     ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E11           1     ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E12           1     ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN

=> s e4
L9            1 "ETHYL 4,4-DIBROMOACETOACETATE"/CN

=> d 19 ide

L9   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   73817-88-6  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Butanoic acid, 4,4-dibromo-3-oxo-, ethyl ester  (CA INDEX NAME)
OTHER NAMES:
CN   Ethyl 4,4-dibromoacetoacetate
MF   C6 H8 Br2 O3
LC   STN Files:   CA, CAPLUS, CASREACT, USPATFULL

http://www.cas.org/legal/infopolicy.html

=> s l9 and l8 and l7
             2 L9
             7 L8
            50 L7
L10          0 L9 AND L8 AND L7
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```
=> s l7 and l8
            50 L7
             7 L8
L11          1 L7 AND L8

=> s l7 and l9
            50 L7
             2 L9
L12          0 L7 AND L9

=> s l8 and l9
             7 L8
             2 L9
L13          0 L8 AND L9

=> d l11 all

L11  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   1959:99446  CAPLUS <<LOGINID::20081229>>
DN   53:99446
OREF 53:17897f-g
ED   Entered STN:  22 Apr 2001
TI   Study of keto-enol equilibrium. γ-Mono-, di- and trihaloacetoacetic
     esters
AU   Loos, H.; Herman, M.
CS   Univ. Ghent
SO   Bulletin des Societes Chimiques Belges (1959), 68, 129-38
     CODEN: BSCBAG; ISSN: 0037-9646
DT   Journal
LA   Unavailable
CC   10B (Organic Chemistry: Aliphatic Compounds)
AB   ClCH2CO2Et (0.5 mole) in Et2O added as rapidly as possible to 0.5 mole Mg
     and an excess of FCH2CO2Et in an equal volume of Et2O gave mixture of
     XCOCH2CO2Et (I) (X = CH2F and = CH2Cl), separated by distillation  Infrared
spectra
     of pure liquid of I (X = Me, CH2F, CHF2, CF3, CH2Cl, CHCl2, and CCl3 are
     recorded, and show bands attributed to C:O (ketonic, ketonic ester, and
     enolic ester), and C:C.  Substitution of F for Cl produces larger
     displacements in wave length and increases in enol content.  I (X = CF3)
     is nearly completely enolized, while I (X = CCl3) has a very low enol
     content, probably due to the steric effect of the Cl atoms.
IT   Isomerism
        (tautomerism, of Et acetoacetate and its halo derivs.)
IT   141-97-9   609-15-4   1522-41-4   16485-10-2
        (Derived from data in the 6th Collective Formula Index (1957-1961))
IT   541-50-4, Acetoacetic acid
        (derivs., enolization of)
IT   352-24-9P, Acetoacetic acid, 4,4-difluoro-, ethyl ester
     372-31-6P, Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester   372-37-2P,
     Acetoacetic acid, 4-fluoro-, ethyl ester   638-07-3P, Acetoacetic acid,
     4-chloro-, ethyl ester   3702-98-5P, Acetoacetic acid, 4,4,4-trichloro-,
     ethyl ester 6082-74-2P, Acetoacetic acid, 4,4-dichloro-, ethyl
     ester
     RL: PREP (Preparation)
        (preparation of)

=> d l11

L11  ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2007:362416  CAPLUS <<LOGINID::20081229>>
DN   148:121227
```

TI Ruthenium catalyzed asymmetric hydrogenation of α- and β-ketoesters in room temperature ionic liquids using chiral P-Phos ligand
AU Xu, Lijin; Lam, Kim Hung; Ruan, Jiwu; Fan, Qinghua; Chan, Albert S. C.
CS Open Laboratory of Chirotechnology of the Institute of Molecular Technology for Drug Discovery and Synthesis and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, Peop. Rep. China
SO ACS Symposium Series (2007), 950(Ionic Liquids in Organic Synthesis), 224-234
CODEN: ACSMC8; ISSN: 0097-6156
PB American Chemical Society
DT Journal
LA English
OS CASREACT 148:121227
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 3 SEA EXA FUL L15

=> d l17 1-3

L17 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 135548-09-3 REGISTRY
ED Entered STN: 16 Aug 1991
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C6 H11 F O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)

L17 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 122666-01-7 REGISTRY
ED Entered STN: 15 Sep 1989
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C6 H11 F O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.

L17 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 122666-01-7 REGISTRY
ED Entered STN: 15 Sep 1989
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C6 H11 F O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.

/ Structure 66 in file .gra /

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 660-47-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Butyric acid, 4-fluoro-3-hydroxy-, ethyl ester (7CI, 8CI)
OTHER NAMES:
CN Ethyl γ-fluoro-β-hydroxybutyrate
CN NSC 24564
MF C6 H11 F O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATOLD
(*File contains numerically searchable property data)

http://www.cas.org/legal/infopolicy.html

=> s l17
L18 6 L17

=> d l18 ibib abs 1-6

L18 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:491670 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 115:91670
ORIGINAL REFERENCE NO.: 115:15755a,15758a
TITLE: Optically active fluorine-containing 3-hydroxybutyric acid esters and process for producing same
INVENTOR(S): Tanida, Kaichi; Suzuki, Yoshiichi
PATENT ASSIGNEE(S): Showa Shell Sekiyu K. K., Japan
SOURCE: Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 427396	A2	19910515	EP 1990-311017	19901008
EP 427396	A3	19920226		
EP 427396	B1	19940914		
R: DE, FR, GB				
JP 03151348	A	19910627	JP 1989-290346	19891108
US 5118836	A	19920602	US 1990-610748	19901108
PRIORITY APPLN. INFO.:			JP 1989-290346 A	19891108

OTHER SOURCE(S): MARPAT 115:91670
AB Optically active ACH(OH)CH2CO2R(I; R = C3-16 alkyl; A = CF3, CHF2, CH2F) are prepared in high optical purity and without racemization by transesterification of inexpensive and easily available Et esters I (R = Et) with an alc. ROH in the presence of an ammonium salts R1SO3- N+HR2R3R4 [R1 = lower alkyl, (un)substituted Ph; R2-R4 = lower alkyl, or NR2R3R4 = pyridine] at 80-150° for 8-15 h. Thus, a mixture of 5.0 g (3R)-CF3CHCOH)CH2CO2R5 (II; R5 = Et) (prepared by stereoselective reduction of CF3COCH2CO2Et with yeast) 25 mL BuOH, 5.0 g pyridinium toluenesulfonate,

and 25 mL PhMe was refluxed at 110° for 3 h and then solvent was removed over 1 h at 120°. Addnl. PhMe and BuOH were added and the procedure repeated to give, after distillation at 62-69°/3 mmHg, II (R5 = Bu). Similarly II (R5 = octyl, hexyl, heptyl) were prepared

L18 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 111:132606
ORIGINAL REFERENCE NO.: 111:22187a,22190a
TITLE: Enzymic manufacture of (R)-γ-substituted-β-hydroxybutyric acid esters
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo; Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-142916 19870608
AB Title esters, useful as intermediates for pharmaceuticals and agrochems., are manufactured by treating γ-substituted acetoacetic acid esters with a NADPH-dependent reductase derived from Sporobolomyces sp. Thus, a mixture of Et γ-chloroacetoacetate, NADPH, and a reductase from Sporobolomyces salmonicolor IFO 1038 was held in a phosphate buffer at pH 6.5 and 28° for 20 h to produce (R)-γ-chloro-β-hydroxybutyric acid Et ester with 98.2% purity and 97% optical purity in 92% yield.

L18 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 110:191289
ORIGINAL REFERENCE NO.: 110:31739a,31742a
TITLE: Enzymic manufacture of γ-substituted β-hydroxybutyrate esters as intermediates for carnitine synthesis
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo; Kato, Masaaki; Morikawa, Tadashi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-145587 19870611
AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ-substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which

form two phases with H2O. Sporobolomyces salmonicolor IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ-chloroacetoacetate, NADPH, and AcOEt at 30° and with pH 8 for 20 h under stirring to produce 92% Et γ-chloro-β-hydroxybutyrate, vs. 52% in the absence of AcOEt.

L18 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:38022 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 56:38022
ORIGINAL REFERENCE NO.: 56:7103i,7104f-i,7105a-d
TITLE: Organic fluorine compounds. XX. Some reactions of 1-chloro-3-fluoropropan-2-ol and epifluorohydrin
AUTHOR(S): Bergmann, Ernst D.; Cohen, Sasson; Shahak, Israel
CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society (1961) 3448-52
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 56:38022

AB cf. CA 55, 9273b.-In 1-chloro-3-fluoropropan-2-ol (I) the Cl atom was much more prone to nucleophilic attack than the F. The reactions with KCN, NaOEt, and NaOPh were studied. Also in epifluorohydrin (II) the oxide ring was opened by diethyl sodiomalonate (III) without attack on the F atom. Alkyl- and arylmagnesium bromide with II gave 1-bromo-3-fluoropropan-2-ol (IV); PhLi gave 1-fluoro-3-phenylpropan-2-ol (V). The preparation of alkyl fluorolactates and fluoropyruvates was described. I (40 g.), 18 g. NaCN, and 10 g. H2O heated 2 hrs. at 50-60° gave 18 g. γ-fluoro-β-hydroxybutyronitrile (VI), b15 125-8°. Dry HCl passed 1 hr. through a refluxing solution of 33 g. VI, 33 g. alc., and 3.5 ml. H2O gave 32 g. Et γ-fluoro-β-hydroxybutyrate (VII), b18 104-8°. P2O5 (10 g.) added portionwise to 16 g. VII in 30 ml. C6H6, the mixture refluxed 15 min., and the decantate distilled gave 7 g. Et γ-fluorocrotonate, b21, 66-7°. II (25 g.) refluxed 2 hrs. in 100 ml. 2N alc. NaOEt gave 6 g. 1-ethoxy-3-fluoro-2-propanol (VIII), b28 71-2°, n29D 1.3995. VIII (31 g.), 41.5 g. Na2Cr2O7, and 70 ml. H2O treated at 15-20° with 69.5 g. H2SO4 and 20 ml. H2O, the mixture, left 2 hrs., extracted with Et2O, and distilled gave 18 g. 1-ethoxy-3-fluoroacetone, b25 63-5°. I (23 g.), 19 g. PhOH, and 8.5 g. NaOH in 70 ml. H2O refluxed gave 28 g. 1-fluoro-3-phenoxypropan-2-ol (IX), b4 110-11°, n30D 1.5138. IX (24 g.) in 70 ml. Me2CO treated at 15-20° with 15 g. CrO3, 23 g. concentrated H2SO4, and 40 ml. H2O and the mixture extracted with Et2O after 3 hrs. gave 17 g. 1-fluoro-3-phenoxyacetone, b4 115-17°, n28D 1.5125. II (38 g.) left 2 hrs. at 40-50° with III from 12 g. Na, 250 ml. alc., and 80 g. diethyl malonate, acidified, evaporated, extracted with Et2O, evaporated, and the residue refluxed 5 hrs. with 100 ml. 10% HCl gave 18 g. δ-fluoro-γ-valerolactone, b32 127-9°, n27D 1.4260. PhLi (from 4 g. Li) in 100 ml. Et2O added in 0.5 hr. at -70° to 19 g. II in 50 ml. Et2O, the temperature raised in 2 hrs. to 0°, and the mixture poured on ice and H2SO4 gave 20 g. V, b15 115-20°. II (14 g.) added dropwise to a Grignard solution (from 2.4 g. Mg and 16 g. PhBr) in 120 ml. Et2O at 0°, the mixture stirred 1 hr., poured on ice and concentrated H2SO4, separated, and distilled gave 7.5 g. IV, b30 78-80°, and 4.5 g.V. 4-Fluoromethyl-2,2-dimethyl-1,3-dioxolane (67 g.), 80 ml. H2O, and 20 ml. concentrated HCl heated and stirred to 80-90°, the mixture refluxed

20 min., distilled, the residue diluted with H2O, warmed 5 hrs. at 60° with 140 ml. 70% HNO3 and 100 ml. H2O, left 48 hrs. at room temperature, heated 1 hr. at 60°, and concentrated, gave fluorolactic acid of 90-5% purity. The sirup distilled azeotropically with 50 g. anhydrous alc., 150 ml. C6H6, and 0.5 g. p-MeC6H4SO3H and the product distilled gave 31-8 g. Et fluorolactate (X), b30 96-8°. Similarly, 59 g. Bu fluorolactate was obtained, b3 94-5°. Azeotropic condensation of 500 g. glycerol and 430 g. EtCOMe in 500 ml. C6H6 in the presence of 20 g. p-MeC6H4SO3H gave 700 g. 2-ethyl-4-hydroxymethyl-2-methyl-1,3-dioxolane (XI), b2 72-3°. XI (146 g.) in 100 ml. C6H6 added to 24 g. NaH in 600 ml. C6H6, the mixture refluxed 0.5 hr., and treated at 25° with 190 g. p-MeC6H4SO2Cl in 300 ml. C6H6 gave the p-tosylate as an oil. The tosylate (300 g.) added to 90 g. KF and 300 ml. O(CH2CH2OH)2, the mixture brought slowly to 150°, left at this temperature 5 min., air passed through 10 min., the distillate dissolved in Et2O, washed, and distilled gave 123 g. 2-ethyl-4-fluoromethyl-2-methyl-1,3-dioxolane, b. 146-7°. X (20.4 g.), 26.7 g. N-bromosuccinimide, and 150 ml. CCl4 refluxed 1 hr. gave 4.5 g. Et fluoropyruvate (XII), b25 82-3°. Reaction of XII with 2,4-dinitrophenylhydrazine gave the 2,4-dinitrophenylhydrazone, m. 125-6°, converted at elevated temperature into Et mesoxaldehyde osazone, m. 250° (AcOH). X (20.4 g.), 53.5 g. N-bromosuccinimide, and 250 ml. CCl4 refluxed 2 hrs. gave 8 g. Et bromofluoropyruvate, b40 100-1°. With 2,4-dinitrophenylhydrazine this compound gave the above osazone. The infrared spectra were given for a number of the above compds.

L18 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:38019 CAPLUS
DOCUMENT NUMBER: 56:38019
ORIGINAL REFERENCE NO.: 56:7104c-e
TITLE: Segregation of organic nitrogen compounds
INVENTOR(S): Fleck, Raymond N.; Wight, Carlyle G.
PATENT ASSIGNEE(S): Union Oil Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2999861		19610912	US 1958-773142	19581112

AB Nonbasic organic N compds. are separated from basic organic N compds. by passage through a Type X mol. sieve adsorbent. The adsorbents are crystalline Type X zeolitic partially dehydrated metallo alumino silicates having pores of substantially uniform diameter of approx. 7-13 A. (Brit. 777,233). The preferred adsorbent is the 13 A. sodium aluminosilicate 6Na2O.6Al2O3.15SiO2 "Molecular Sieves 13X." The preferred adsorbent at approx. 265°F. is treated with a 1:1 mixture of hydrocarbons and organic N compds. from a hydrogenated shale oil coker distillate. The N-containing portion of the mixture is approx. 76% (by weight) basic N compds. and 24% nonbasic N compds. After liquid phase treatment 6 hrs., the adsorbent is separated from the raffinate which contains substantially all of the hydrocarbon and some of the N compds. The N-containing portion is approx. 97% (by weight) basic N compds. and 3% nonbasic N compds. The absorbent is treated with a displacement exchange fluid such as pyridine to give an extract whose N-containing fraction, when separated from pyridine, is approx. 73% basic N compds. and 27% nonbasic N-compds. Similarly, vapor phase treatment is carried out at about 550°F.

L18 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:38018 CAPLUS
DOCUMENT NUMBER: 56:38018
ORIGINAL REFERENCE NO.: 56:7104a-c
TITLE: Diesters
INVENTOR(S): Quaedvlieg, Mathieu; Boehmke, Guenther
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1115027		19611012	DE 1958-F25347	19580326

AB Diesters are prepared from dicarboxylic acids with one free OH group. Thus, a surface active polyglycol ether 2000 prepared from 40 moles ethylene oxide and 1 mole diphenyl ethyl phenol is mixed at 80-100° with maleic anhydride 49 dissolved in toluene 100 parts. After 0.5 hr. p-toluenesulfonic acid 5 parts is added to the mixture and the temperature raised to 120-30° to distil the H2O and most of the toluene. The remaining toluene is distilled in vacuo and the p-toluenesulfonic acid neutralized with an equivalent amount of concentrated NaOH. The dicarboxylic acid diester produced is used as a dispersing agent. Similar diesters are prepared from phthalic acid anhydride, succinic acid anhydride, and adipic acid.

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6 L17
44 L13
L19 2 L17 AND L13

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L19 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 111:132606
ORIGINAL REFERENCE NO.: 111:22187a,22190a
TITLE: Enzymic manufacture of (R)-γ-substituted-β-hydroxybutyric acid esters
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo; Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-142916 19870608

AB Title esters, useful as intermediates for pharmaceuticals and agrochems., are manufactured by treating γ-substituted acetoacetic acid esters with a NADPH-dependent reductase derived from Sporobolomyces sp. Thus, a mixture

of Et γ-chloroacetoacetate, NADPH, and a reductase from Sporobolomyces salmonicolor IFO 1038 was held in a phosphate buffer at pH 6.5 and 28° for 20 h to produce (R)-γ-chloro-β-hydroxybutyric acid Et ester with 98.2% purity and 97% optical purity in 92% yield.

IT 95310-94-4P 122666-01-7P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, with reductase of Sporobolomyces and NADPH)

RN 95310-94-4 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 68 in file .gra /

RN 122666-01-7 CAPLUS
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 69 in file .gra /

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L19 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 111:132606
ORIGINAL REFERENCE NO.: 111:22187a,22190a
TITLE: Enzymic manufacture of (R)-γ-substituted-β-hydroxybutyric acid esters
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo; Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-142916 19870608

AB Title esters, useful as intermediates for pharmaceuticals and agrochems., are manufactured by treating γ-substituted acetoacetic acid esters with a NADPH-dependent reductase derived from Sporobolomyces sp. Thus, a mixture of Et γ-chloroacetoacetate, NADPH, and a reductase from Sporobolomyces salmonicolor IFO 1038 was held in a phosphate buffer at pH 6.5 and 28° for 20 h to produce (R)-γ-chloro-β-hydroxybutyric acid Et ester with 98.2% purity and 97% optical purity in 92% yield.

IT 95310-94-4P 122666-01-7P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)

(manufacture of, with reductase of Sporobolomyces and NADPH)
RN 95310-94-4 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 70 in file .gra /

RN 122666-01-7 CAPLUS
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 71 in file .gra /

L19 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 110:191289
ORIGINAL REFERENCE NO.: 110:31739a,31742a
TITLE: Enzymic manufacture of γ-substituted β-hydroxybutyrate esters as intermediates for carnitine synthesis
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo; Kato, Masaaki; Morikawa, Tadashi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		
PRIORITY APPLN. INFO.:			JP 1987-145587	19870611

AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ-substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which form two phases with H2O. Sporobolomyces salmonicolor IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ-chloroacetoacetate, NADPH, and AcOEt at 30° and pH 8 for 20 h under stirring to produce 92% Et γ-chloro-β-hydroxybutyrate, vs. 52% in the absence of AcOEt.
IT 660-47-9P, Ethyl γ-fluoro-β-hydroxybutyrate
32224-01-4P, Ethyl γ-bromo-β-hydroxybutyrate
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, enzymic, from acetoacetate derivative, two-phase system in)
RN 660-47-9 CAPLUS
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 72 in file .gra /

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RN   32224-01-4  CAPLUS
CN   Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester  (CA INDEX NAME)

http://www.cas.org/legal/infopolicy.html

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             2 L33
            38 L34
           145 L35
L36          0 L33 AND L34 AND L35

=> s l33 and (or l34) and (or l35)
MISSING TERM 'AND (OR'
The search profile entered contains a left parenthesis,
'(' followed by an operator.

=> s l34 and l35
            38 L34
           145 L35
L37          5 L34 AND L35

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L37  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2004:353051  CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER:          140:374010
TITLE:                    Preparation of optically active alcohols from ketones
                          using Daucus carota tuber extract
INVENTOR(S):              Yadav, Jhillu Singh; Nanda, Samik; Reddy, Polepally
                          Thirupathi; Rao, Adari Bhaskar
PATENT ASSIGNEE(S):       Council of Scientific and Industrial Research, India
SOURCE:                   U.S. Pat. Appl. Publ., 11 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    --------------------   --------
     US 20040082043       A1    20040429    US 2002-282066         20021029
     US 7056540           B2    20060606
PRIORITY APPLN. INFO.:                      US 2002-282066         20021029
OTHER SOURCE(S):          CASREACT 140:374010
AB   The present invention relates to an enzymic process for the preparation of
     optically active chiral alcs. using tuberous root Daucus carota ;
     particularly invention relates to an enzymic process for the preparation of
     optically active alcs. by enantioselective reduction of corresponding ketones
     using tuberous root Daucus carota.
TI   Preparation of optically active alcohols from ketones using Daucus carota
     tuber extract
REFERENCE COUNT:          1     THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
IT   1445-91-6P   1517-67-5P   1572-97-0P, S-1-(4-Methoxyphenyl)-ethanol
     4221-99-2P   6033-23-4P   14898-80-7P 16493-60-0P   20107-40-8P
     25501-32-0P   26184-62-3P   33401-74-0P   51154-54-2P,
     S-1-(4-Methylphenyl)-ethanol   52019-78-0P   53732-47-1P   56816-01-4P
     61586-79-6P 85571-85-3P   86728-85-0P   93781-59-0P,
     S-1-(4-Hydroxyphenyl)-ethanol   95537-36-3P   96156-72-8P,
     S-1-(4-Nitrophenyl)-ethanol   99528-42-4P, S-1-(4-Chlorophenyl)-ethanol
     100760-04-1P, S-1-(4-Bromophenyl)-ethanol   101219-73-2P,
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S-1-(4-Fluorophenyl)-ethanol 112653-32-4P 120523-15-1P 134625-72-2P
169272-21-3P 169272-22-4P 169272-23-5P 169436-90-2P 297765-54-9P
341513-45-9P 341513-46-0P 438528-24-6P 438528-26-8P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP
(Preparation)
(preparation of optically active alcs. from ketones using Daucus carota
tuber extract)

L37 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:886005 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 137:369737
TITLE: Stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors
INVENTOR(S): Tada, Kenichi; Miura, Takashi
PATENT ASSIGNEE(S): Takasago International Corporation, Japan
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 13
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1258470	A2	20021120	EP 2002-291172	20020510
EP 1258470	A3	20030813		
EP 1258470	B1	20050817		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003034665	A	20030207	JP 2002-82865	20020325
JP 4015450	B2	20071128		
ES 2247280	T3	20060301	ES 2002-291172	20020510
US 20030004362	A1	20030102	US 2002-142983	20020513
US 6723871	B2	20040420		
PRIORITY APPLN. INFO.:			JP 2001-150012 A	20010518
			JP 2002-82865 A	20020325
OTHER SOURCE(S):	CASREACT 137:369737; MARPAT 137:369737			

GI

/ Structure 95 in file .gra /

AB Optically active β-hydroxycarboxylate esters R1CH(OH)CH2CO2R2 [R1 = C1-10 (un)branched perfluoroalkyl or perchloroalkyl; R2 = C1-8 lower alkyl, (un)substituted benzyl; e.g., optically active Et 4,4,4-trifluoro-3-hydroxybutanoate] are prepared in high yield and selectivity by stereoselective hydrogen transfer to the corresponding β-ketocarboxylate esters R1COCH2CO2R2 (e.g., Et 4,4,4-trifluoro-3-oxobutanoate) in the presence of hydrogen donors (e.g., formic acid-triethylamine mixts.) and a chiral ruthenium-diamine complex catalyst [I; * = asym. carbon atom; R3, R4 = alkyl, Ph, (un)substituted cycloalkyl; R5 = methanesulfonyl, trifluoromethanesulfonyl, benzenesulfonyl, (un)substituted naphthyl, camphorsulfonyl, alkoxycarbonyl, (un)substituted benzoyl; R6 = H, alkyl; A = (un)substituted aromatic compound; X = halogen; e.g., RuCl[(1R,2R)-p-TsNHCH(C6H5)CH(C6H5)NH2] (p-cymene)].

TI Stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate

esters from β-ketocarboxylate esters and hydrogen donors
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
IT 372-30-5P, Ethyl 4,4,4-trifluoro-3-hydroxybutanoate
19486-93-2P, Ethyl 4,4,4-trichloro-3-hydroxybutanoate
305322-80-9P, Isopropyl 4,4,4-trifluoro-3-hydroxybutanoate
475467-53-9P, Methyl 4,4,4-trifluoro-3-hydroxybutanoate
475467-55-1P, Methyl 3-hydroxy-4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-pentadecafluorodecanoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β-hydroxycarboxylate esters from β-ketocarboxylate esters and hydrogen donors)

L37 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:326792 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 137:46794
TITLE: Efficient enantioselective reduction of ketones with Daucus carota root
AUTHOR(S): Yadav, J. S.; Nanda, S.; Reddy, P. Thirupathi; Rao, A. Bhaskar
CORPORATE SOURCE: Organic Division, Indian Institute of Chemical Technology, Hyderabad, 500007, India
SOURCE: Journal of Organic Chemistry (2002), 67(11), 3900-3903
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:46794
AB A novel and efficient reduction of various prochiral ketones such as acetophenones, α-azido aryl ketones, β-keto esters, and aliphatic acyclic and cyclic ketones to the corresponding optically active secondary alcs. with moderate to excellent chemical yield was achieved by using Daucus carota, root plant cells under extremely mild and environmentally benign conditions in aqueous medium, has been described. Many of these optically active alcs. are the potential chiral building blocks for the synthesis of pharmaceutically important mols. and asym. chiral ligands. Hence, this biocatalytic approach is found to be the most suitable for the preparation of a wide range of chiral alcs. and gave inspiration for the development of a new biotechnol. process.
TI Efficient enantioselective reduction of ketones with Daucus carota root
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
IT 1445-91-6P 1517-67-5P 1572-97-0P 4221-99-2P 6033-23-4P
14898-80-7P 16493-60-0P 20107-40-8P 25501-32-0P
26184-62-3P 27544-18-9P 33401-74-0P 51154-54-2P 52019-78-0P
53732-47-1P 56816-01-4P 61586-78-5P 61586-79-6P 85571-85-3P
86728-85-0P 93781-59-0P 95537-36-3P 95537-41-0P 96156-72-8P
99528-42-4P 100760-04-1P 101219-73-2P 112653-32-4P 119341-64-9P
120523-15-1P 134625-72-2P 169272-21-3P 169272-22-4P 169272-23-5P
169436-90-2P 297765-54-9P 341513-45-9P 341513-46-0P 438528-24-6P
438528-25-7P 438528-26-8P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(enantioselective reduction of ketones with Daucus carota root)

L37 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:559159 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 115:159159
ORIGINAL REFERENCE NO.: 115:27255a,27258a

TITLE: Preparation of pyrimidine derivatives as herbicides
INVENTOR(S): Hatanaka, Masataka; Watanabe, Junichi; Kondo, Yasuo; Suzuki, Koichi; Nawamaki, Tsutomu; Watanabe, Shigeomi
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03031266	A	19910212	JP 1989-164942	19890627
PRIORITY APPLN. INFO.:			JP 1989-164942	19890627

OTHER SOURCE(S): MARPAT 115:159159
GI

/ Structure 96 in file .gra /

AB Pyrimidine derivs. [I; R = H, (substituted) alkyl, alkali metal ion, alkaline earth metal ion, NH4, R1, R2 = halo, alkyl, alkoxy, haloalkyl, haloalkoxy, dialkylamino; X1, X2, Y1, Y2 = H, cyano, carboxy, CHO, alkoxycarbonyl, alkoxy, (substituted) alkyl, etc.] are prepared NaH (55% oil) was added to a solution of MeCH(OH)CHMeCO2Et and sulfone II is THF under cooling and the mixture was stirred at room temperature to give 93% I (R = Et, R1 = R2 = MeO, X1 = Y1 = H, X2 = Y2 = Me), which killed >90% barnyard grass, large crabgrass, etc. at 25.0 g/are.
TI Preparation of pyrimidine derivatives as herbicides
IT 372-30-5P 32328-03-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of herbicide)
IT 105-50-0 383-63-1 1587-15-1 19487-29-7 55107-14-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of herbicide)

L37 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:184695 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 102:184695
ORIGINAL REFERENCE NO.: 102:28965a,28968a
TITLE: Preparation by yeast reduction and determination of the sense of chirality of enantiomerically pure ethyl (-)-4,4,4-trichloro-3-hydroxy- and (+)-4,4,4-trifluoro-3-hydroxybutanoate
AUTHOR(S): Seebach, Dieter; Renaud, Philippe; Schweizer, W. Bernd; Zueger, Max F.
CORPORATE SOURCE: Lab. Org. Chem., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Helvetica Chimica Acta (1984), 67(7), 1843-53
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:184695
GI

/ Structure 97 in file .gra /

AB Reduction of EtO2CCH2COCR3 (R = Cl, F) by fermenting baker's yeast (Saccharomyces cerevisiae) on a preparation scale (20-50 g in .apprx.3L H2O) gave 70-80% EtO2CCH2CH(OH)CR3 (I) with 85% ee (ee = enantiomeric excess) (-)-(S)-I (R = Cl) and 45% ee of (-)-(R)-I (R = F). Recrystn. of I (R = Cl, F) or their 3,5-(O2N)2C6H3CO2 esters gave >98% ee. The absolute configurations of I were determined The x-ray crystal structure of the ester from (+)-(R)-I (R = F) and (-)-camphanoyl chloride, II, was determined
TI Preparation by yeast reduction and determination of the sense of chirality of enantiomerically pure ethyl (-)-4,4,4-trichloro-3-hydroxy- and (+)-4,4,4-trifluoro-3-hydroxybutanoate
IT 372-30-5P 95605-60-0P 95615-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
IT 85571-85-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and esterifications of, use of yeast in)
IT 16493-60-0P 16493-64-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, hydrolysis, and esterifications of, use of yeast in)


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=> s l12 and l6
          448 L12
           88 L6
L13        37 L12 AND L6

=> d l13 ibib abs hitstr 1-5

L13  ANSWER 1 OF 37  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2008:1383615  CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER:         149:512458
TITLE:                   Enantioselective reduction of ketones
AUTHOR(S):               Itsuno, Shinichi
CORPORATE SOURCE:        Toyohashi University of Technology, Toyohashi, Japan
SOURCE:                  Organic Reactions (Hoboken, NJ, United States) (1998),
                         52, No pp. given
                         CODEN: ORHNBA
                         URL: http://www3.interscience.wiley.com/cgi-
                         bin/mrwhome/107610747/HOME
PUBLISHER:               John Wiley & Sons, Inc.
DOCUMENT TYPE:           Journal; General Review; (online computer file)
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 149:512458
AB   A review of the article Enantioselective reduction of ketones.
IT   86728-93-0P 86728-99-6P 88496-70-2P
     90835-93-1P 90866-33-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (Enantioselective Reduction of Ketones)
RN   86728-93-0  CAPLUS

L13  ANSWER 2 OF 37  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2008:1116154  CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER:         149:531428
TITLE:                   Engineering of NADPH-dependent aldo-keto reductase
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from Penicillium citrinum by directed evolution to improve thermostability and enantioselectivity
AUTHOR(S): Asako, Hiroyuki; Shimizu, Masatoshi; Itoh, Nobuya
CORPORATE SOURCE: Organic Synthesis Research Laboratory, Sumitomo Chemical Co., Ltd., 1-98, Kasugade-naka 3-chome, Konohana-ku, Osaka, 554-8558, Japan
SOURCE: Applied Microbiology and Biotechnology (2008), 80(5), 805-812
CODEN: AMBIDG; ISSN: 0175-7598
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Penicillium citrinum β-keto ester reductase (KER) can catalyze the reduction of Me 4-bromo-3-oxobutyrate (BAM) to Me (S)-4-bromo-3-hydroxybutyrate with high optical purity. To improve the thermostability of KER, protein engineering was performed using error-prone polymerase chain reaction-based random mutagenesis. Variants with the highest levels of thermostability contained the single amino acid substitutions L54Q, K245R, and N271D. The engineered L54Q variant of KER retained 62% of its initial activity after heat treatment at 30°C for 6 h, whereas wild-type KER showed only 15% activity. The L54Q substitution also conferred improved enantioselectivity by KER. An Escherichia coli cell biocatalyst that overproduced the L54Q mutant of KER and glucose dehydrogenase as a cofactor regeneration enzyme showed the highest level of BAM reduction in a water/butyl acetate two-phase system.
IT 86728-85-0P, S-Ethyl 4-chloro-3-hydroxybutyrate 88759-56-2P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(engineering of NADPH-dependent aldo-keto reductase from Penicillium citrinum by directed evolution to improve thermostability and enantioselectivity)
RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L13 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:757902 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 149:221820
TITLE: Asymmetric reduction of substituted α- and β-ketoesters by Bacillus pumilus Phe-C3
AUTHOR(S): He, Chunmao; Chang, Dongliang; Zhang, Jie
CORPORATE SOURCE: Guangzhou Institute of Chemistry, Chinese Academy of Sciences, Guangzhou, 510650, Peop. Rep. China
SOURCE: Tetrahedron: Asymmetry (2008), 19(11), 1347-1351
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The enantioselective reduction of substituted α- and β-ketoesters using resting cells of Bacillus pumilus Phe-C3 was investigated. Effects of substrate concentration on the catalytic efficiency of the microorganism were studied. Preparative scale productions were carried out under the optimized conditions with 62.4-91.0% yields and 90.2-97.1% ee. The cells retained 80% of initial activity after recycling for six times.
IT 86728-85-0P, Ethyl (S)-4-chloro-3-hydroxybutyrate 95537-36-3P
RL: BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)

(asym. reduction of substituted α- and β-ketoesters by Bacillus pumilus Phe-C3)
RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

L13 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1101864 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 148:10703
TITLE: A practical and efficient procedure for reduction of carboxylic acids and their derivatives: use of KBH4-MgCl2
AUTHOR(S): Qiu, You-Chun; Zhang, Fu-Li; Zhang, Chun-Nian
CORPORATE SOURCE: Pharmacochemistry Division, Shanghai Institute of Pharmaceutical Industry, Shanghai, 200437, Peop. Rep. China
SOURCE: Tetrahedron Letters (2007), 48(43), 7595-7598
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:10703
AB The use of KBH4-MgCl2 to reduce carboxylic acids and their derivs. to the corresponding alcs. or the resp. reduced products is described. Me (S)-3,4-O-isopropylidene-3,4-dihydroxybutanoate used as a reference substrate was reduced with KBH4 and MgCl2 in 1:1 mol ratio to 80 % (S)-1,2-O-isopropylidene-1,2,4-butanetriol. KBH4-LiCl gave higher yields but LiCl is more expensive than MgCl2.
IT 86728-85-0, Ethyl (3S)-4-chloro-3-hydroxybutanoate
95537-36-3, Ethyl (3S)-4-bromo-3-hydroxybutanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(practical and efficient procedure for reduction of carboxylic acids and their derivs. using KBH4-MgCl2)
RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L13 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:873237 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 147:277913
TITLE: Improved method and kit for automated resolving agents, especially amino acid derivatives, and solvents selection
INVENTOR(S): Vaidya, Niteen A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 29pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070185346	A1	20070809	US 2006-347532	20060203
WO 2007092264	A2	20070816	WO 2007-US2800	20070131
WO 2007092264	A3	20071129		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,

KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
EP 1981831 A2 20081022 EP 2007-763121 20070131
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
PRIORITY APPLN. INFO.: US 2006-347532 A2 20060203
WO 2007-US2800 W 20070131

AB The invention is related to a kit for improved identification of the optimal conditions for diastereomeric salt crystallization and the selection of the optimal resolving agents, especially amino acid derivs., and solvents, which include A. an array of containers wherein the array is a standard high throughput tray and the containers are a multiplicity of substantially identical containers or well plates each optionally sealed with a sealant or stoppers to avoid loss of chemical solvent; B. wherein each substantially identical container has a unique combination of resolving agent in each column and at least one suitable solvent in each row; and C. an instructional text to use said kit. The tray of 24, 48, 96 or more samples is examined simultaneously visually or by standard anal. techniques. Resolution of (±)-2-phenylpropionic acid was studied with both amines and acids as resolving agents. Strychnine in 96% ethanol was ideal system for (+)-isomer, while quinidine in 96% ethanol was the system of choice for (-)-isomer. Pyroglutamic acid in 70% isopropanol was ideal system for (+)-isomer, while malic acid in in 1-butanol was the system of choice for (-)-isomer.

IT 10488-69-4, Ethyl 4-chloro-3-hydroxybutyrate 32224-01-4, Ethyl 4-bromo-3-hydroxybutyrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolving agent; method and kit for automated resolving agents, especially from amino acid derivs., and solvents selection)

RN 10488-69-4 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 150 in file .gra /

RN 32224-01-4 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 151 in file .gra /

=> d l13 ibib abs hitstr 30-37

L13 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 111:132606
ORIGINAL REFERENCE NO.: 111:22187a,22190a
TITLE: Enzymic manufacture of (R)-γ-substituted-β-hydroxybutyric acid esters
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;

Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		
PRIORITY APPLN. INFO.:			JP 1987-142916	19870608

AB Title esters, useful as intermediates for pharmaceuticals and agrochems., are manufactured by treating γ-substituted acetoacetic acid esters with a NADPH-dependent reductase derived from Sporobolomyces sp. Thus, a mixture of Et γ-chloroacetoacetate, NADPH, and a reductase from Sporobolomyces salmonicolor IFO 1038 was held in a phosphate buffer at pH 6.5 and 28° for 20 h to produce (R)-γ-chloro-β-hydroxybutyric acid Et ester with 98.2% purity and 97% optical purity in 92% yield.

IT 86728-99-6P 88496-70-2P 90866-33-4P
95310-94-4P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, with reductase of Sporobolomyces and NADPH)

RN 86728-99-6 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 152 in file .gra /

RN 88496-70-2 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 153 in file .gra /

RN 90866-33-4 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 154 in file .gra /

RN 95310-94-4 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 155 in file .gra /

L13 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:439010 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 111:39010
ORIGINAL REFERENCE NO.: 111:6633a,6636a

TITLE: Preparation of β-hydroxyalkanoate esters as synthetic intermediates
INVENTOR(S): Sayo, Noboru; Akutagawa, Susumu; Saito, Takao; Noyori, Ryoji; Kumobayashi, Hidenori; Takaya, Hidemasa
PATENT ASSIGNEE(S): Takasago International Corp., Japan
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 295109	A1	19881214	EP 1988-305293	19880609
EP 295109	B1	19920304		
EP 295109	B2	19960904		
R: CH, DE, FR, GB, LI, NL				
JP 63310847	A	19881219	JP 1987-145975	19870611
JP 06099367	B	19941207		
US 4933482	A	19900612	US 1988-204480	19880609
PRIORITY APPLN. INFO.:			JP 1987-145975 A	19870611

OTHER SOURCE(S): MARPAT 111:39010
GI

/ Structure 156 in file .gra /

AB Optically active R1CHOHCHR3COR2 (R1 = alkyl; CF3, aryl; R2 = alkoxy, alkylthio, PhS, R4R5N where R4,R5 = H, alkyl, PhCH2; R3 = H, halo, alkyl, alkoxycarbonyl, alkoxycarbonylalkyl; R1R3 = to form a 4- to 6-membered alicyclylic) are prepared by asym. hydrogenation of R1COCHR3COR2 in the presence of a ruthenium-optically active phosphine complex. A mixture of MeCOCH2CO2Me, MeOH, H2O, and Ru2Cl4[(+)-I]2(NEt3) (R = H) (preparation given) was autoclaved at 30° and 40kg/cm2 H to give 98% Me (3R)-(-)-3-hydroxybutyrate (99.1% optical purity).
IT 10488-68-3P 109462-45-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by hydrogenation of ketocarboxylate)
RN 10488-68-3 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester (CA INDEX NAME)

/ Structure 157 in file .gra /

RN 109462-45-5 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, methyl ester (CA INDEX NAME)

/ Structure 158 in file .gra /

L13 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 110:191289
ORIGINAL REFERENCE NO.: 110:31739a,31742a
TITLE: Enzymic manufacture of γ-substituted β-hydroxybutyrate esters as intermediates for carnitine synthesis
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;

Kato, Masaaki; Morikawa, Tadashi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-145587 19870611

AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ-substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which form two phases with H2O. Sporobolomyces salmonicolor IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ-chloroacetoacetate, NADPH, and AcOEt at 30° and pH 8 for 20 h under stirring to produce 92% Et γ-chloro-β-hydroxybutyrate, vs. 52% in the absence of AcOEt.

IT 10488-68-3P, Methyl γ-chloro-β-hydroxybutyrate
10488-69-4P, Ethyl γ-chloro-β-hydroxybutyrate
32224-01-4P, Ethyl γ-bromo-β-hydroxybutyrate
86728-85-0P, Ethyl (S)-γ-chloro-β-hydroxybutyrate
90866-33-4P, Ethyl (R)-γ-chloro-β-hydroxybutyrate
117935-49-6P, Octyl γ-chloro-β-hydroxybutyrate
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, enzymic, from acetoacetate derivative, two-phase system in)

RN 10488-68-3 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester (CA INDEX NAME)

3 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:6366 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 110:6366
ORIGINAL REFERENCE NO.: 110:1195a,1198a
TITLE: Preparation of L-carnitine by microbial reduction of acetoacetic acid derivatives and chemical derivatization
INVENTOR(S): Sih, Charles J.
PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite SpA, Italy
SOURCE: U.S., 11 pp. Cont.-in-part of U.S. Ser. No. 544,957
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4710468	A	19871201	US 1984-580439	19840215
US 4642290	A	19870210	US 1982-447171	19821206
AU 8321758	A	19840614	AU 1983-21758	19831128
AU 566906	B2	19871105		
CA 1225956	A1	19870825	CA 1983-442170	19831129
IL 70352	A	19871020	IL 1983-70352	19831130

FI 8304419	A	19840607	FI 1983-4419		19831202
FI 81115	B	19900531			
FI 81115	C	19900910			
CH 661498	A5	19870731	CH 1983-6448		19831202
DK 8305592	A	19840607	DK 1983-5592		19831205
DK 163917	B	19920421			
DK 163917	C	19920914			
NO 8304461	A	19840607	NO 1983-4461		19831205
NO 159291	B	19880905			
NO 159291	C	19881214			
SE 8306714	A	19840607	SE 1983-6714		19831205
SE 455501	B	19880718			
SE 455501	C	19881110			
GB 2132614	A	19840711	GB 1983-32359		19831205
GB 2132614	B	19860326			
ZA 8309038	A	19840725	ZA 1983-9038		19831205
AT 8304237	A	19910115	AT 1983-4237		19831205
AT 393136	B	19910826			
DE 3344085	A1	19840607	DE 1983-3344085		19831206
DE 3344085	C2	19931014			
FR 2537130	A1	19840608	FR 1983-19505		19831206
FR 2537130	B1	19881014			
NL 8304190	A	19840702	NL 1983-4190		19831206
JP 59118093	A	19840707	JP 1983-230449		19831206
JP 07067674	A	19950314	JP 1993-217710		19930901
PRIORITY APPLN. INFO.:			US 1982-447171	A2	19821206
			US 1983-544957	A2	19831021

OTHER SOURCE(S): CASREACT 110:6366; MARPAT 110:6366

AB L-Carnitine is prepared from γ-substituted amides or esters of acetoacetic acid by a stereospecific microbial reduction followed by chemical derivatization steps. γ-Chloroacetoacetic acid octyl ester in Tween 80 was added to an actively growing culture of Candida kefyr and incubated for 24 h. The product, 4-chloro-3(R)-hydroxybutyric acid octyl ester (I), was isolated from the broth supernatant in .apprx.70% yield by chromatog. on silica gel. I (1.5 g) was heated with Me3N in 3 mL EtOH for 2 h to yield a solid that was heated in 10% HCl at 80-90° for 1.5 h. After evaporation of the solvents, 320 mg L-carnitine chloride was extracted from the residue with EtOH and precipitated with ether.

IT 86728-97-4 86728-98-5 86729-01-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)

RN 86728-97-4 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, hexyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 165 in file .gra /

RN 86728-98-5 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, heptyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 166 in file .gra /

RN 86729-01-3 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, decyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 167 in file .gra /

IT 88496-70-2P 90866-33-4P 108100-49-8P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, by microbial reduction of acetoacetate, for carnitine manufacture)
RN 88496-70-2 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 168 in file .gra /

RN 90866-33-4 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 169 in file .gra /

RN 108100-49-8 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, 1,1-dimethylethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 170 in file .gra /

IT 86728-99-6P 90835-93-1P 90835-94-2P
90835-97-5P 90835-98-6P 91990-59-9P
RL: PREP (Preparation)
(preparation of, microbial, for carnitine manufacture)
RN 86728-99-6 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 171 in file .gra /

RN 90835-93-1 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 172 in file .gra /

RN 90835-94-2 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 173 in file .gra /

RN 90835-97-5 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, propyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 174 in file .gra /

RN 90835-98-6 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, butyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 175 in file .gra /

RN 91990-59-9 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, phenylmethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 176 in file .gra /

L13 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:596550 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 107:196550
ORIGINAL REFERENCE NO.: 107:31521a,31524a
TITLE: Optically active α-halo-β-hydroxybutyrate manufacture by Saccharomyces species
INVENTOR(S): Hasegawa, Masayasu; Okada, Shigetaka; Hamada, Nobutake; Sakai, Kiyofumi; Honda, Hiroshi
PATENT ASSIGNEE(S): Nippon Synthetic Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62126997	A	19870609	JP 1985-268811	19851128
US 4933282	A	19900612	US 1986-935199	19861126
PRIORITY APPLN. INFO.:			JP 1985-268811 A	19851128

OTHER SOURCE(S): CASREACT 107:196550
AB γ-Haloacetoacetic acid esters are reacted with a Saccharomyces species to obtain optically active γ-halo-β-hydroxybutyric acid esters. Thus, S. cerevisiae IFO 0635 was shake-cultured in YM medium for 48 h. The cells were collected and incubated with a mixture containing 0.8 g glucose and 1 g Et γ-chloroacetoacetate at 27° for 3 h to give Et γ-chloro-β-hydroxybutyrate with .apprx.75% conversion.
IT 10488-69-4P, Ethyl γ-Chloro-β-hydroxybutyrate
109462-45-5P, Methyl γ-Bromo-β-hydroxybutyrate
110930-70-6P, Allyl γ-Chloro-β-hydroxybutyrate
110930-71-7P, Benzyl γ-Chloro-β-hydroxybutyrate
110930-72-8P, Octyl γ-Bromo-β-hydroxybutyrate
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, from haloacetoacetate, by Saccharomyces)
RN 10488-69-4 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 177 in file .gra /

RN 109462-45-5 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, methyl ester (CA INDEX NAME)

/ Structure 178 in file .gra /

RN 110930-70-6 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, 2-propen-1-yl ester (CA INDEX NAME)

/ Structure 179 in file .gra /

RN 110930-71-7 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, phenylmethyl ester (CA INDEX NAME)

/ Structure 180 in file .gra /

RN 110930-72-8 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, octyl ester (CA INDEX NAME)

/ Structure 181 in file .gra /

L13 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:32369 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 106:32369
ORIGINAL REFERENCE NO.: 106:5415a,5418a
TITLE: Asymmetric reduction of β-keto esters
INVENTOR(S): Ai, Kenzo
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61155354	A	19860715	JP 1984-281337	19841227

PRIORITY APPLN. INFO.: JP 1984-281337 19841227

AB R1COCH2CO2R2 (R1, R2 = alkyl, alkenyl, alkynyl, aryl, aralkyl, etc.) are asym. reduced in the presence of [R3NR5CHR4(CH2)mY]n (R3, R5 = H, amino-protecting group, R3R5N = heterocycle; R4 = CO2H, CH2OH; m = 0-3; Y = SH, OH, NH2, CO2H when n = 1; Y = S when n = 2) and C1-20 alcs., PhOH, benzyl alc. etc. Thus, LiBH4 was added to a solution of 1.21 mmol (R,R)-N,N'-dibenzoylcystine and 1.61 mmol Me3COH in THF, refluxed, cooled, 1.01 mmol PhCOCH2CO2Et added, and the mixture stirred at -30° to give 94% (R)-(+)-PhCH(OH)CH2CO2Et of 87% optical yield.

IT 32224-01-4P 90866-33-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 32224-01-4 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 182 in file .gra /

RN 90866-33-4 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 183 in file .gra /

L13 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:130396 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 102:130396
ORIGINAL REFERENCE NO.: 102:20453a,20456a
TITLE: On the steric course of baker's yeast mediated reduction of alkyl 4-azido- and 4-bromo-3-oxobutyrate. Synthesis of (R)- and (S)-carnitine
AUTHOR(S): Fuganti, Claudio; Grasselli, Piero; Casati, Paolo; Carmeno, Massimo
CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, 20133, Italy
SOURCE: Tetrahedron Letters (1985), 26(1), 101-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:130396
AB Bakers' yeast reduction of Et 4-azido- and 4-bromo-3-oxobutyrate affords (3R) and (3S) carnitines, resp., in high optical purity.
IT 86728-85-0 86728-99-6 95537-36-3
RL: PROC (Process)
(transformation of, by bakers' yeast, stereospecificity in)
RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 184 in file .gra /

RN 86728-99-6 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 185 in file .gra /

RN 95537-36-3 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 186 in file .gra /

L13 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:437206 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 101:37206
ORIGINAL REFERENCE NO.: 101:5813a,5816a
TITLE: L-Carnitine and its intermediate products
INVENTOR(S): Sih, Charles J.
PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite S.p.A., Italy
SOURCE: Belg., 38 pp.

CODEN: BEXXAL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 898396	A1	19840330	BE 1983-212002	19831206
US 4642290	A	19870210	US 1982-447171	19821206
AU 8321758	A	19840614	AU 1983-21758	19831128
AU 566906	B2	19871105		
CA 1225956	A1	19870825	CA 1983-442170	19831129
IL 70352	A	19871020	IL 1983-70352	19831130
FI 8304419	A	19840607	FI 1983-4419	19831202
FI 81115	B	19900531		
FI 81115	C	19900910		
CH 661498	A5	19870731	CH 1983-6448	19831202
DK 8305592	A	19840607	DK 1983-5592	19831205
DK 163917	B	19920421		
DK 163917	C	19920914		
NO 8304461	A	19840607	NO 1983-4461	19831205
NO 159291	B	19880905		
NO 159291	C	19881214		
SE 8306714	A	19840607	SE 1983-6714	19831205
SE 455501	B	19880718		
SE 455501	C	19881110		
GB 2132614	A	19840711	GB 1983-32359	19831205
GB 2132614	B	19860326		
ZA 8309038	A	19840725	ZA 1983-9038	19831205
AT 8304237	A	19910115	AT 1983-4237	19831205
AT 393136	B	19910826		
DE 3344085	A1	19840607	DE 1983-3344085	19831206
DE 3344085	C2	19931014		
FR 2537130	A1	19840608	FR 1983-19505	19831206
FR 2537130	B1	19881014		
NL 8304190	A	19840702	NL 1983-4190	19831206
JP 59118093	A	19840707	JP 1983-230449	19831206
JP 07067674	A	19950314	JP 1993-217710	19930901
PRIORITY APPLN. INFO.:			US 1982-447171 A	19821206
			US 1983-544957 A	19831021

AB L-Carnitine [541-15-1] is prepared from γ-substituted amides or esters of acetoacetic acid by a stereospecific microbial reduction followed by chemical derivatization steps. Thus, γ-chloroacetoacetic acid octyl ester [41051-21-2] in Tween 80 was added to an actively growing culture of Candida kefyr and incubated for 24 h. The product, 4-chloro-3(R)-hydroxybutyric acid octyl ester (I) [86728-99-6], was isolated from the broth supernatant in .apprx.70% yield by chromatog. on silica gel. I (1.5 g) was heated with Me3N [75-50-3] in 3 mL EtOH for 2 h to yield a solid that was heated in 10% HCl at 80-90° for 1.5 h. After evaporation of the solvents, 320 mg L-carnitine chloride [6645-46-1] was extracted from the residue with EtOH and precipitated with ether.

IT 86728-97-4 86728-98-5 86729-01-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)

RN 86728-97-4 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, hexyl ester, (3R)- (CA INDEX NAME)